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AIR POLLUTION: PROCEEDINGS OF THE MEETING OF THE EXPERT PANEL ON AIR POLLUTION MODELING (4th), HELD IN OBERURSEL, WEST GERMANY ON 28-30 MAY 1973

NATO Committee on the Challenges of Modern Society

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PROCEEDINGS OF THE FOURTH MEETING OF THE EXPERT PANEL ON AIR POLLUTION MODELING

A Report of the Air Pollution Pilot Study,
NATO Committee on the Challenges of Modern Society

Oberursel, Federal Republic of Germany
May 28-30, 1973

OTHER NATO/CCMS AIR POLLUTION PUBLICATIONS

Technical Report on the Conference on Low Pollution Power Systems Development, N. 4

Proceedings of the Second Meeting of the Expert Panel on Air Pollution Modeling, N. 5

Guidelines to Assessment of Air Quality (Revised) SO_x, TSP, CO, HC, NO_x and Oxidants, N. 6*

Air Quality Criteria for Sulfur Oxides, N. 7*

Air Quality Criteria for Particulate Matter, N. 8*

Air Quality Criteria for Carbon Monoxide, N. 10*

Proceedings of the Third Meeting of the Expert Panel on Air Pollution Modeling, N. 14

Air Quality Criteria for Nitrogen Oxides, N. 15

*Also available in French

These documents may be obtained from the NATO Committee on the Challenges of Modern Society, 1110 Bruxelles, Brussels, Belgium, or from the Air Pollution Technical Information Center, Office of Air and Water Programs, Environmental Protection Agency, Research Triangle Park, North Carolina 27711, U.S.A. (English only).

PREFACE

The primary objective of the 4th Meeting of the NATO/CCMS Expert Panel on Air Pollution Modeling was to stimulate maximum informal exchange of technical information, on several topics currently considered to be of major interest and importance in air quality simulation modeling. Encouraged by the success of the 3rd Meeting held 2-3 October, 1972, in Paris, France, and to allow exchange of ideas on a broad international basis, the participation at the meeting extended far beyond the regular membership countries. It included representatives and observers from W. Germany, U.S.A., Canada, U.K., France, Sweden, Norway, Denmark, Netherlands, Belgium, Italy, Australia, Israel, Greece and Czechoslovakia.

In contrast to the 3rd Meeting, for which participants were invited to submit prepared papers, the 4th Meeting comprised a series of five workshop sessions and extended over three whole days. The present document provides a brief summary of the several workshop discussions and the introductory remarks of the chairmen of the sessions, together with some papers that were variously prepared as back-up information for the workshops.

K. L. Calder, Acting Chairman
NATO/CCMS Expert Panel on Air Pollution Modeling
Chief Scientist, Meteorology Laboratory
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PROCEEDINGS OF THE FOURTH MEETING OF THE EXPERT PANEL ON AIR POLLUTION MODELING

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Chapter I

NATO Committee on the Challenges of Modern Society

AIR POLLUTION

Agenda for 4th Meeting of the Expert
Panel on Air Pollution Modeling

Oberursel, W. Germany
28-30 May, 1973

AGENDA

4th Meeting of NATO/CCMS Expert Panel on Modeling

Oberursel, W. Germany, 28-30 May, 1973

Monday 28 May: 0930-1230 hrs and 1430-1730 hrs

Workshop on Applications of Modeling and Users' Needs

Discussion leaders:

Dr. K. Jones, Environmental Protection Agency, U.S.A.

Dr. Ing F. J. Dreyhaupt, Ministerium für Arbeit, Gesundheit und Soziales L.N.W., Dusseldorf, W. Germany

Tuesday 29 May: 0930-1230 hrs.

Workshop on Validation of Air Quality Simulation Models

Discussion leader:

Prof. Dr. H. Fortak, Institute for Theoretical Meteorology, Free University of Berlin, W. Germany

Tuesday 29 May: 1430-1700 hrs

Workshop on the Role of Regional Air Pollution Studies in Model Development

Discussion leader:

Prof. Dr. W. Klug, Technische Hochschule Darmstadt, W. Germany

Wesnesday 30 May: 0930-1230 hrs

Workshop on the Role of Empirical-Statistical Modeling of Air Quality

Discussion leader:

Dr. N. Busch, Danish Atomic Energy Commission, Denmark

Wednesday 30 May: 1400-1430 hrs

Workshop on Simplicity Versus Sophistication in Air Quality Modeling

Discussion leader:

Dr. F. A. Gifford, National Oceanic and Atmospheric Administration, U.S.A.

Chapter II

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4th Meeting NATO/CCMS Expert Panel on
Air Pollution Modeling

Oberursel, W. Germany
28-30 May, 1973

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Chapter III

OPENING REMARKS

by

K. L. Calder

4th Meeting NATO/CCMS Expert Panel on
Air Pollution Modeling

Oberursel, W. Germany

28-30 May, 1973

OPENING REMARKS

It gives me great pleasure to see so many familiar faces around these tables and particularly as our last meeting was only a little over six months ago. As the acting chairman for this 4th Meeting of the NATO/CCMS Expert Panel on Modeling, I would like to welcome you all. I must also convey to you the sincere regrets of the chairman, Mr. R. A. McCormick, that he will not be able to be present. However, we are fortunate in having with us for this meeting Dr. K. Jones who is the U. S. Director of the CCMS air pollution project, as well as many other distinguished representatives and experts from the international air quality modeling community.

The last meeting of the CCMS Panel on Modeling held in Paris on 2-3 October 1972 was intentionally enlarged well beyond the regular Panel membership. This was in order to accommodate a broader objective and to encourage a maximum exchange of ideas on a wide front. The meeting involved many of the most active contributors in the field of air quality modeling. It seemed to have been quite enthusiastically received and to have met its prime objective of stimulating a wide exchange of technical information. At a brief meeting following the concluding technical discussions, and attended by the official members of the Panel, it was unanimously agreed to recommend another wide-participation meeting in the late spring of 1973. It was also agreed that in contrast to the 3rd Meeting, for which participants had been invited to prepare and present technical papers, the 4th Meeting should be organized along the lines of a discussion workshop. This would be of three days duration and centered around just five carefully chosen special topics in order to allow sufficient time for discussions in depth. Five such topics were suggested by me in a February 1973 letter addressed to all previous participants, and it appears that these suggestions met with general approval. The first two topics relating to applications of modeling and users' needs, and the validation of air quality simulation models, were in fact lightly touched upon during the discussions in Paris. The other three topics on the role of regional air pollution studies in model development, on the role of empirical/statistical modeling of air quality, and what I rather ambiguously called "Simplicity versus sophistication in air quality modeling," also appear to be of great interest at the present time. In fact, all seem to be of sufficiently wide interest that the five workshops will be held consecutively so as to permit attendance of all of them by those desiring to do so. To reflect its unusual overall importance, the whole of today will be spent on the 1st workshop topic of applications of modeling and users' needs. We are fortunate that Dr. Kay Jones of the U. S. Environmental Protection Agency and Dr. F. Dreyhaupt of the Ministerium fur Arbeit, Gesundheit and Soziales, Dusseldorf, have agreed to act as co-leaders for the discussion of this workshop. Discussion leaders for the other workshops sessions are Professor Heinz Fortak from the Free University of Berlin, Professor Werner Klug from the Technische Hochschule Darmstadt, Dr. Niels Busch from the Danish Atomic Energy Commission and Dr. Frank Gifford from the U. S. National Oceanic and Atmospheric Administration. I would like to thank all of these gentlemen in advance for so generously agreeing to lead our discussions and so ensure the success of this 4th Panel Meeting.

For two of our previous meetings proceedings have been published under the CCMS project, that contained the papers that were presented and some additional discussion. No prepared papers were solicited for the present meeting although discussion leaders were invited to open up their topics with a 15-30 minute presentation at the beginning of each session. It is hoped, nevertheless, that sufficient technical information will be developed from these sessions and exchanges that it will be worthwhile putting this on permanent record through a proceedings of this 4th Meeting. While open to any suggestions on this matter, I would like to propose that participants and speakers during the next three days be prepared to submit to me informal notes of their remarks and contributions to the discussion before the close of the day on Wednesday 30 May. Alternatively, if this should not be possible perhaps participants will be agreeable to sending their remarks to me not later than, say, 30 June 1973. These will then be consolidated with the introductory remarks of the workshop leaders to form a permanent record of the information exchange at the meeting.

Last, but not least, I would like to call upon Dr. von Hesler of the Regional Planning Office, Frankfurt, in case he has any announcements that should be made. Dr. von Hesler has been associated with the CCMS air pollution project from its inception and has made all the administrative arrangements for this meeting. At this time I would also like to circulate a list, which I know must be incomplete, of the names and affiliations of many who were invited to attend this meeting. Will you please examine this list very carefully and check for the detail of your own entry. If your name and address is not there please add it on the separate sheet that I am also circulating.

For our general benefit and information, and following Dr. von Hesler's announcements, Dr. Kay Jones of the U. S. Environmental Protection Agency has agreed to briefly describe the origin and history of the CCMS air pollution project and will also mention some of the plans for the future. After this, we will start our first workshop session. This will be jointly led by Dr. K. Jones and Dr. F. Dreyhaupt and occupy us for the remainder of the day.

Before starting the workshop session, it will be nice to go around the table and introduce ourselves by name and affiliation.

Chapter IV

Summary of Workshop Discussions*

K. L. Calder, Meteorology Laboratory
Environmental Protection Agency, U.S.A.

4th Meeting of NATO/CCMS Panel on Modeling

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* The author takes this opportunity of thanking several of the participants for responding to the invitation to mail to him a written statement of their contribution to the discussion.

APPLICATIONS OF MODELS AND USERS' NEEDS

Dr. Kay Jones, U.S. Director of the NATO/CCMS Air Pollution Project co-chaired the first day's meeting with Dr. F. J. Dreyhaupt of the Federal Republic of Germany, for a workshop on the above theme. Before introducing the workshop session (see Chapter V) Jones briefly reviewed the history of the CCMS Air Pollution Project. In the area of air quality modeling the effort had started in 1969-70 with efforts to apply models for Ankara, Frankfurt and St. Louis, although this had rapidly grown to include Rotterdam, Oslo, Milan, Turin and Haifa. He indicated that although it was now planned to terminate the CCMS Air Pollution Project in the spring of 1974, because of its marked success it was intended to continue the activity of the Expert Panel on Modeling, and probably with increased emphasis on applied considerations. The formal mechanisms for the continuation had yet to be worked out. In all probability the FRG will assume the leadership as a new CCMS initiative. It is anticipated that the modeling panel will meet annually or possibly semi-annually in the future, and the next meeting will probably be held late this fall.

Dr. Jones then addressed himself to the workshop topic and stated that in his opinion there was a serious communications problem between the model developers and users of models, such as air quality management decision makers. Such lack of communications produces many adverse manifestations, e.g., misuse of modeling results, lack of confidence in applying useful models, insufficient dedication of resources to model development, etc. An important matter for consideration at the workshop should be how to bridge this gap between modeler and user. He thought it was up to the modelers to provide users with a good indication of the limitations and accuracy of each model and, furthermore, in terms that the users could understand. Turner (U.S.A.) said that a recognition of this communications problem was to be found in the existence of a Model Applications Branch as well as a Model Development Branch, within the Meteorology Laboratory of the U.S. Environmental Protection Agency. The first group was primarily concerned with applications and adapting existing models to meet special users' needs. It developed computer programs and users' manuals for fairly wide distribution. They advised users by close contacts, e.g., by telephone, and were intending to use the mechanism of two-day workshops, with each devoted to a specific model, to provide understanding on how to use models to the users. Turner also referred to the Users' Network for Applied Modeling of Air Pollution (UNAMAP). This was a recently established teleprocessing network that made available a number of current air quality simulation models to both EPA and non-EPA users. The models involved are all in the form of computer programs accessible at remote user terminals that are connected to the central EPA IBM 360/50 computer facility by regular telephone lines. Some of the models that are so available at present are (1) HIWAY - A model that calculates pollutant concentration in the vicinity of a roadway. (2) SRI Urban Diffusion Model - A short-term model that calculates the automotive contribution to carbon monoxide levels. (3) CDM (Climatological Dispersion Model) - A long-term (seasonal and annual) model that calculates sulfur dioxide and particulate levels from point and area sources in an urban area. The use of these models by remote terminals requires only a minimum of programming knowledge. Some models can be executed "on-line" by a user who interactively enters the control parameters specific to his problem (e.g., wind speed and direction, source strength, stack height, etc.). Other models require more extensive input data that involves developing a data set separate from the program. Turner suggested that user workshops on some of these models might be useful within the CCMS framework.

Kwizak (Canada) said that he agreed with Dr. K. Jones that the NATO/CCMS modeling meetings emphasizing applied programs (to avoid duplication with other agencies such as WMO, OECD, etc.), have been a useful forum for the exchange and consolidation of the current state of the knowledge in urban pollution modeling. Also, they have stimulated research activities to develop new techniques in regional and urban pollution modeling. In particular, there have been useful spin-offs to other countries, including Canada, from the pilot studies conducted in the cities of St. Louis, Ankara, Oslo, Rotterdam, Frankfurt, Milan, etc.

These studies have not only provided useful data and techniques in the application of dispersion models but they have contributed also to air quality management, formulation of air quality criteria, and th[illegible] enhancement of our knowledge in control technology. They have a[illegible] brought into proper focus the importance of meteorology to the user[illegible] As Canada's representative, he believed that the NATO/CCMS air pollution modeling activities should continue until the spring of 1974, since there is still so much excellent unfinished research work being conducted which should be completed. He would strongly suggest that, in the reappraisal of the NATO/CCMS activities by the central organization, serious consideration be given to the amalgamation of the CCMS air pollution working group and the active modeling panel, into one group. This new group should continue its activities beyond the spring of 1974. Some of the problems that will require serious future consideration by such a group are as follows:

(a) The coming development of advanced automative power systems of (pollution-less) vehicles will need evaluation to avoid replacing present pollutants and their inherent problems with other problems possibly involving new and unknown contaminants.

(b) The communications gap between the modeler and the user is a serious one and needs to be bridged. The erroneous use of present models through misapplication, the lack of understanding of the importance of meteorological parameters, the need for more sophisticated and accurate urban and regional models, and the fact that the user needs answers today, all have contributed to poor results which frequently have led to questionable policy decisions in environmental management.

(c) A user-modeler interface workshop should be pursued vigorously, not only to educate the user but also to educate the modeler. The participants should include (in Canada's case at least), a modeler, a federal government user, and a typical provincial government user.

Since it is imperative that the communications gap between the modeler and the user be reduced, he would support Dr. Kay Jones in suggesting that U.S.A., as a pilot country, convene a modeler-user meeting in the fall of 1973 or early in 1974. Finally, he believed that the present membership of this panel should decide for their own countries, the typical federal and provincial (or state) users who should be invited to such a meeting or workshop.

Barrett (U.K.) said that the decision makers who would benefit from our models occur at different levels of government (and outside it!) - e.g., in different parts of central government and in local authorities. Obtaining a representative cross-section may be a matter of some difficulty. It seemed to him that the functions of the meeting should be not only to diffuse information to decision makers but also to assist us to understand more clearly their requirements and to learn better how to put across to them what models can do. This is particularly important because it seems unlikely that the message can be gotten across in one meeting covering many countries with different governmental structures. Most of the work will have to be done by modelers in individual countries.

Neumann (Israel) agreed that it is highly desirable that we should work toward a better understanding by potential users of the value and limitations of models. But, it is equally important, he felt, to achieve a closer rapport among modelers coming from different disciplines and, especially, among those belonging to different organizations. In some cases there is very little cooperation and understanding among the modelers themselves, a fact which does not enhance the confidence of users in the models. He thought it was appropriate to quote here the words of a cabinet minister: "Whenever I have to make an important decision, I call in two experts. They will surely disagree and then I make my own decisions."

Keddie (U.K.) said that definition of "user" is difficult and we have found that very close contact between the modeler and user (of information obtained from the model) is essential. The modeler must also be responsible for his predictions and be prepared to give the limits of accuracy.

Every effort should be made to ensure that technical arguments do not occur between modelers during the proposed modeler-user working session. Such conflict would almost certainly confuse the users present and perhaps destroy what faith they may already have in modeling.

Schneider (Netherlands) mentioned that in some cases he thought that the modelers were asked the wrong questions and Olsson (Sweden) said that he thought modelers should be included in the planning committees. Dreyhaupt (W. Germany) said that he thought the decision makers (users) wanted to make the decisions and not have these made by the modelers, although Fortak (W. Germany) felt that gaps between the modelers and decision makers sometimes forces the modeler to make the decisions.

Olsson (Sweden) indicated that regional dispersion models are at various stages of development for three urban regions (Stockholm, Malmö-Lund and Gothenburg) in Sweden. Attempts are being made to take users needs into account in the development phases of the models. Project committees, where representatives from regional planning groups as well as industries participate, have been formed and meet on a regular basis. It is felt that an improved mutual understanding of the problems facing the modeler as well as the potential users, have been achieved through these committees. The most serious problems noted might be the modelers inability to clearly demonstrate the relative value of various model-types and the validity of any one model. These problems are closely related to the validity problem and will be discussed later.

On the other hand there is a lack of properly formulated criteria (although the recommended SO_2 criteria used in Sweden seem to be rather well formulated for model applications) and an apparent inability on the part of the user to appreciate the relative merits and limitations inherent in the model results. We have to accept that the models available are far from perfect, although in most cases will already give us a better estimate of the air quality situation than any other method available. There is a need for improved ways of communication and means of bringing about a better understanding between the modelers and the various user groups.

Velds (Netherlands) mentioned that a round-table meeting between modelers and users was to be held in June in the Netherlands. It should be possible to report on the results next year. He felt that sometimes the users ask for results with much greater accuracy than the modelers can provide. Gifford (U.S.A.) considered that it was desirable for the modelers to make any simplifications that might be possible in their models and not leave this to somebody else. He also felt that in many cases field studies should be conducted in order to make the models more accurate, and that for some situations, as in complex terrain, this field data was required to validate the modeling activities. . Hessler (W. Germany) felt that perhaps it was better to develop some rough and approximate models immediately, and without waiting a long time for perfection.

In continuing the same workshop discussion after the lunch-break, Dr. F.J. Dreyhaupt (W. Germany) first referred to the fact that at the 3rd Meeting of the Panel on Modeling he had promised a report on the Cologne pilot scheme for establishing an inventory of atmospheric pollutants. He then distributed a most lavishly produced report "Emissionskataster Köln" that had been published on this subject in December 1972, by the Minister of Labor, Health and Social Affairs of North Rhine and Westphalia, together with an English translation (see Chapter XVIII). He then went on to present, in a comprehensive fashion, his ideas on the role of air quality simulation models in strategic plans for air pollution control (see Chapter XI).

Turner (U.S.A.) then presented a paper entitled "Users' Needs and the Applications of Air Quality Simulation Models" that had been specially written to provide background material for the workshop (see Chapter XIV). He described the variety of users of modeling in the U.S.A. and their various needs, and then briefly discussed several general types of models that were currently in use or under development. These were mentioned under the headings: stable pollutants from isolated point sources, stable pollutants from multiple sources, concentrations from mobile sources, and models for photochemical pollutants. He emphasized that adequate models are not available at the present time for situations of complex topography, for stagnation conditions where the winds are extremely light and variable, or for the photochemical air pollution problem. Gifford (U.S.A.) again pointed to the need for experimental tests for complex terrain and mentioned some experiments being conducted by the National Oceanic and Atmospheric Administration, with sulphur hexafluoride as a tracer, at Huntington Canyon, Utah, U.S.A. These were to determine the flow effects and concentrations in complex terrain. He pointed to the need for a clear differentiation of those situations which may be amenable to modeling, from those which cannot.

Kwizak (Canada) said that there is a need for large scale models to handle areas such as from Detroit to Quebec. He considered that these will only be achieved through meteorological-pollutant prediction models that analyze the meteorology and pollutant transport simultaneously, and of type similar to those now used for weather prediction. There seemed to be general agreement on the need for these more sophisticated meso-scale dynamical meteorological models, while the discussion also emphasized the difficulties of meteorological prediction for modeling.

Jones (U.S.A.) returned to the question he had raised in the morning session of how best to implement the modeler-user interface. The discussion during the day had only emphasized the urgent need for such a meeting. Schneider (Netherlands) suggested that the compilation of a list of models with guidelines for their use in specific cases, and recommendations for their modification, where appropriate, for other applications would be very useful. Olsson (Sweden) said that he thought such a meeting should emphasize how to interrelate with the users and clarify the users' needs, rather than be an attempt to educate the users on models and their limitations. Jones (U.S.A.) concluded the discussion with suggestions to establish the protocol for a modeler-user forum in the fall. The protocol would be drafted by the pilot country (U.S.A.) and circulated to the attendees for comment, in addition to key users (yet to be determined) in the NATO member governments. General papers would be prepared on the status of currently applied models as well as user needs. A synthesis of these papers by the pilot country would determine the priorities for discussions and demonstrations of model applications at the next panel meeting. He anticipated that this meeting would be scheduled for later this fall and it should be restricted to no more than 50 or 60 total attendees to insure effective discussion.

VALIDATION OF AIR QUALITY SIMULATION MODELS

This subject had also been a topic at the 3rd Meeting of the Panel on Modeling, and had been considered sufficiently important to merit a more extended discussion. Professor H. Fortak (W. Germany) opened up the discussion (see Chapter VI) by describing the validation procedure that he had adopted for his Bremen model. This was a statistical model, not in the sense of generating a time series, but as providing the ensemble of concentration fields corresponding to all the meteorological conditions that occurred during the time period of interest. In validating the model the pollution concentration frequency distribution, for half-hour averaged values of the ensemble, was calculated at strategically chosen locations and compared with measured values. The most critical test of the model is when the statistics are compared for each wind direction separately. It is natural that the differences in this test are larger than when a comparison is made without separation of wind directions, although the differences in the case of Bremen were relatively small. He suggested testing climatological models of urban air pollution by means of such wind roses. Fortak also mentioned the much more difficult task of validating time-dependent models, where the simulation might suffer from lack of knowledge of the initial conditions. Such validation would need to recognize the stochastic nature of the prediction and would involve modern concepts from sampling theory.

In the ensuing discussion Gifford (U.S.A.) asked what complexity had entered into the urban models that frequently caused larger variations in the calculated values (larger maximum and lower minimum) than in the measurements. Although a ready answer was not forthcoming Neumann (Israel) pointed out that most models are steady-state, whereas the atmosphere is usually in transition and has not reached a steady state. We, therefore, tended to overestimate and underestimate concentrations by changing them too rapidly in the models. Olsson (Sweden) thought that we saw more variability from a model than from observation primarily because the use of hourly wind data results in a wind with less inertia than the actual wind. Fox (U.S.A.) felt that this was an effect of using an incorrect wind field as much as anything else. We needed to consider the spatial and temporal variability in the wind and temperature fields over the entire region under consideration. Otherwise we are responding to turbulent fluctuations in the field, that is to say, turbulence on a larger scale if the measurements represent an hourly average. He felt that since more complete meteorological knowledge leads to quite variable winds, this variation should be included, even to arrive at averaged results. Neumann (Israel) also referred to the great spatial and temporal variations of conditions that can obtain in mesometeorological flows, as for instance, in areas strongly affected by sea, or lake and land breezes, and by other local circulations. Since many large cities are situated on sea or lake coasts, the matter is of some importance. He said that even Dr. Lars Olsson, who comes from a city located in a high geographic latitude where the sea breezes would be expected to be of limited significance, has commented on the effect of sea breezes in the Stockholm area on pollutant concentration. If we are not sufficiently aware of some of the changing and changeable nature of features of these local circulations, we may draw incorrect conclusions concerning turbulent diffusion and pollutant emissions or concentrations. To illustrate the foregoing point, he showed four slides relating to a recent theoretical study (by Y. Mahrer and himself, at the Dept. of Atmospheric Sciences, The Hebrew University of Jerusalem) of the sea-and land-breeze circulation over level islands of 50 km radius. The slides show how this circulation evolves from an assumed state of rest, how the flow system intensifies and progresses inland. A sea-breeze front forms and instabilities in the flow lead to the formation of a (shallow) pressure low about the front, complete with its own circulation system, horizontal convergences and divergences of the wind both near the surface and "aloft", vertical motions, etc. The front does not just progress but intensifies in the process up to some time in the afternoon when the vertical transfer of heat from the now cooling land surface no longer supplies enough energy to feed the developing circulation about the front. If we apply the equation for the rate of change of turbulent kinetic energy to the conditions predicted for the horizontal convergence area just behind the sea-breeze front, we find that it is an area of enhanced rate of "production" of turbulent energy. If we are not aware of these dynamic developments, we might interpret the relatively low pollution concentrations expected to prevail in the area of intensified turbulence behind the front, as a lowering of emission rates. More generally, the slides suggest that flow conditions (and pollutant concentrations) can vary considerably over relatively short distances in such mesometeorological systems.

Olsson (Sweden) commented that the models under development for urban regions are based on the Gaussian diffusion model, in the manner described by Fortak. The limitations of this model, especially under "low wind" conditions, are well known and are the reason that other types of models are being considered, such as the continuity equation type of model developed by Grønskei for Oslo. The models for Stockholm and Malmö-Lund have been tested against four months of hourly and 24-hourly data, for several stations located in the two regions. Autocorrelation coefficients, RMSQ values, etc., have been calculated, as well as log-normal frequency distributions, in attempts to validate the models. The most difficult question seems to be related to the quality and representativeness of the air quality data e.g., the accuracy of the SO_2 concentration measurements and the question of point measurements relative to calculated grid area-averages. May be the best way to validate a planning model was to examine frequency distributions, for example, by using Larsen's log-normal model or a pollution wind rose as is done by Fortak. By keeping all but one parameter constant the relative importance of the various submodels could be tested, as was suggested by Johnson at the 3rd NATO/CCMS meeting. Olsson indicated that he had found in this way that the model is most sensitive to variations in wind speed and mixing height, and also had a wind-directional boundary-flux dependence. Further analyses might indicate the relative importance of these various submodels and how the model as a whole could be optimized. Serious problems are related to the inaccuracies of the emission inventories, as the model output is strongly dependent on temporal and spatial variations of the latter.

Barrett (U.K.) inquired whether it was the general feeling, as Olsson had expressed, that models should be validated in parts as Johnson had earlier suggested. Fox (U.S.A.) warned that, based on his experience with photochemical modeling, the verification of the parts of a model might be quite inadequate if the information comes from different situations. He pointed out that often the photochemical models resulted in good validation statistics for ozone, in spite of the NO - NO_2 trends being incorrect. He argued that validation should be based on a proper physical basis. Often we are required to develop models in great haste so that very gross approximations must be made. However, we should attempt to improve these models, not primarily under the criterion of obtaining results that look better, but rather in the direction of improved physical understanding and description.

Grønskei (Norway) said that in addition to a statistical validation, a test of the model under different specified meteorological conditions should be included. This would provide information on the abilities of the different models to describe air pollution in areas having different climatologies. At the Norwegian Institute for Air Research they would support the proposal of Dr. Olsson to select areas as test areas for different air pollution models. They would be willing to organize the observational data from the Oslo study so as to make them suitable for testing different air pollution models.

Olsson (Sweden) referred to the need in model development, for instruments that would provide concentration values integrated over some path length, so as to provide measurements that could be compared more directly with the area-averaged values referred to in Professor Fortak's opening remarks. Smith (U.K.) indicated that in some cases these averaged values could be of greater interest as, for example, in determining the exposure dose for a person traveling in a moving vehicle.

Busch (Denmark) emphasized that sometimes, in averaging, we may be averaging out the effects of numerous errors in the model, such as the neglect of wind direction shear with height. He also stated that the use of empirical factors, such as a half-life for SO_2, is sometimes equivalent to crude calibration of the model without proper regard for the physics. He also mentioned a power plant study in Denmark to investigate the physical and chemical transformations of SO_2. This was a European Community Program.

Kropp (W. Germany) summarized a paper (see Chapter XII) that described the air pollution model that had been developed for Cologne. This had been referred to on the previous day by Dr. F. J. Dreyhaupt.

THE ROLE OF REGIONAL AIR POLLUTION STUDIES IN MODEL DEVELOPMENT

This discussion was introduced (see Chap. VII) by Professor Klug (W. Germany) who began by inquiring whether there was any agreement as to what constituted a regional study. There was much discussion on this question. Keddie (U.K.) thought that the extent of the region might depend on the pollutant being considered, while Busch (Denmark) suggested that the scale might be that over which advection dominates over diffusion. Smith (U.K.) indicated that the horizontal dimensions of an area; which we can call a Region and for which we can develop a Regional pollution study, may lie between limits set by two meteorological properties. The lower limit is given by that horizontal distance beyond which ground-level concentrations are significantly affected by the depth of the mixing layer. Typically during the daytime this is of the order of 20 km downwind from the source area. This limit separates Regional pollution problems from urban pollution problems provided the urban areas are relatively compact and do not sprawl over considerable areas. The upper limit is given by the typical length scale over which meteorological parameters are relatively uniform, i.e., over some fraction of the synoptic-scale. Analysis of 24-hour average sulfur dioxide concentrations at rural sites in Britain suggests that the inter-site concentration correlations remain fairly steady up to about 200 km and then fall significantly. The upper limit may be set therefore around 200 km. A region so defined would require a model which takes into account the source distribution in a rather broad sense, the depth of the mixing layer (and its temporal variation), meso-scale circulations and topography, but characteristically assumes uniformity in geostrophic wind, cloud amount and vertical temperature structure. Grønskei (Norway) also supported the notion that the meteorological processes that need to be included should give content to the concept of a regional air pollution model. He proposed to include air pollution problems that have a typical length and time scale for which meso-meteorological processes need to be considered. On a regional spatial scale a multitude of pollution sources, located in different areas, will often have to be taken into account. As for the time scale, chemical transformations and cleansing processes in the atmosphere should be considered in addition to the meteorological processes.

In spite of the variety of considerations that were involved there seemed to be a concensus of opinion that urban studies would involve distances of the order of 10 km while for regional studies the length scale would be of the order of 100 km.

Fox (U.S.A.) described (see Chap. XIII) the current status of the Regional Air Pollution Study (RAPS) of the U.S. Environmental Protection Agency. Gifford (U.S.A.) also mentioned that two regional pollution studies were being conducted by the U.S. Atomic Energy Commission in the Upper Mississippi Valley and the Tennessee Valley, and indicated the importance of deposition, washout and decay for such studies. Rusch (Denmark) also expressed the need for a more precise understanding of those physical processes, such as advection, scavenging and cloud physics, that may be of importance.

Keddie (U.K.) stated that the survey-modeling study in Central Scotland, mentioned at the 3rd Meeting in Paris, is now underway. The size of the area under detailed study is about 20 km x 35 km and therefore fits into the lower end of the regional scale suggested by Professor Klug. The area contains a mixture of urban and small and large scale industrial developments but these cover only about 40% of the ground, the remainder being mainly open country. The purpose of the study is to provide information on the current distribution of smoke and sulfur dioxide, quantify the contributions from the various types of source (residential, commercial and industry) to the observed concentrations and from sources outside the survey area (e.g. the cities of Glasgow and Edinburgh), and predict the impact of new industrial and residential developments within the area.

Eighteen daily monitoring stations are being set up to provide information on the distribution of the two pollutants and to validate the model to be developed. Some of the instruments have been located at points where concentrations are expected to be most sensitive to any changes in the emissions from major industrial sources and others have been located so as to provide the most information on the transport of pollution into and out of the area. Some fourteen additional monitoring instruments will be operated by local authorities and industry as part of the UK National Survey. Meteorological data will be obtained from three airports on the perimeter of the area and, in addition, wind speed and direction will perhaps be measured at one or two locations within the study area. The emission inventors will be on a 1 km square grid basis. The study is intended to last for a period of about 2 years.

There is certainly a pressing need for models capable of application to "regional scales". However, the use of the word "region" is confusing in this context because the model developer will have his own view while the planner will almost certainly have another. Perhaps the best choice of scale is the one which is compatible with the physics of these larger scale models.

Olsson (Sweden) indicated that regional dispersion models were in various stages of development for three regions in Sweden (Stockholm, Malmö-Lund, and Gothenburg). In regional air pollution studies there is a great need for good air-quality data but these need to be paired with good meteorological measurements. He felt that it was generally more profitable to invest in a few high quality representative stations than in large networks. This is not to say that we do not need studies like RAPS and METROMET. On the contrary we need to learn much more about urban meteorology, local and mesoscale interactions, and their relationship to air pollution dispersion, as a basis for further development of physically sound models.

Keddie (U.K.), Barrett (U.K.) and Olsson (Sweden) all expressed great interest in remote sensing techniques, such as lidar and sonar, both for meteorological and air quality observations, and emphasized their importance for regional modeling studies.

Olsson (Sweden) said there was a need for "test city type" sets of data that could be used by modelers to compare different types of models or various modifications for any one model. He suggested that this subject be taken up at the next NATO/CCMS meeting, and that possibly the "make up" and "administration" of such sets of data could be discussed. Olsson (Sweden) and Fox (U.S.A.) also discussed the idea of using the RAPS data to establish a set of test data, against which models might be compared critically. Some thoughts on such a data bank were that (1) it should be in the form of magnetic tape of such density that it could be read by any reasonable computer, (2) data should be for about 30 days, with 20 of these days of high concentration measurements, (3) data should be available, as at least 1-hour averages, for wind speed and direction at station, stability from the best information, and pollutant concentrations, and (4) emission inventory estimates should be available on a 1-hour basis.

Fox (U.S.A.) expressed his view that meteorological field modeling, that included as much physics as we knew for a given situation knew, would represent the next step in the development of an improved modeling capability. In this he was strongly supported by Kwizak (Canada) who said that he felt that meteorological prediction for control can be achieved using the Navier-Stokes equations and treating meteorology and pollution in the atmosphere as one problem. By 1985 he did not think we could or would desire to separate the two. He felt that a concerted effort is needed to develop new and better models which should be based on the solution of the Navier-Stokes equations by finite differences, and which included the physical and chemical processes of pollutants. Technology for the development of such models exists and handling the regional and urban models can be accomplished by the use of nested grids. While existing dispersion models are very good, we have reached a plateau in our methodology, due to the limited applicability of these models, which is usually to the site of the plant environment. However, for the present we must continue to rely on statistical, qualitative, and on plant-site dispersion models supplemented with considerable information on local mesoscale meteorology (e.g. wind stability, temperature, effects of terrain and bodies of water, etc.). The development of new models as part of meteorological models is the only way in which we will be able to make predictions of air quality extending out to one or two days, and even for larger periods of time. A paper by Kwizak, that develops these ideas further, is included as Chap. XVII in these Proceedings. Busch (Denmark) alluded to the difficulty of verifying meso-scale models and said that he felt there might be some advantage in first looking for a simple model that identified all the factors of controlling importance. Gifford (U.S.A.) pointed to the need for scale analysis in modeling and particularly when this was to include chemical reactions.

THE ROLE OF EMPIRICAL/STATISTICAL MODELING OF AIR QUALITY

In his introductory remarks Dr. N. Busch (Denmark) referred to some ideas of Calder relating to the possibility of developing a source-oriented empirically-based air quality simulation model in contrast to the usual models that required as an *a priori* input a meteorological dispersion formulation (see Chapter VIII). He then suggested that in order to avoid semantic difficulties an *ad hoc* approach should be adopted for the workshop discussion, and that any considerations that related to the statistical aspects of air simulation modeling would be regarded as appropriate. Busch then mentioned three types of statistical models: (1) the purely statistical ones where a prediction is attempted without any knowledge of the detailed physics of the problem, (2) traditional objective forecast methods that involve utilization of existing data, and (3) regression type models, and in particular analysis by the use of empirical orthogonal functions. He was working on the orthogonal function approach, which is closely related to ordinary regression analysis. This method might serve a useful purpose if, with more regard to the physics of the pollution problem, some kind of physical arguments could be produced that would make it possible to categorize a pollution concentration field in terms of a small number of meteorological categories, e.g., wind speed, wind direction, time of day, etc. The basic idea then was that within each of these categories the concentration distribution would show a characteristic pattern as displayed by the eigenfunctions. In this way, it might be possible to establish an air pollution climatology in terms of the expansion coefficients and the categories. This could be useful in detecting changes in typical pollutant patterns that would indicate changes in source distribution, so that in this sense the approach would be source-oriented.

Kwizak (Canada) alluded to the use of orthogonal functions in meteorological analysis, that dated back to the first application by Lorenz in 1956, and in which there had been great progress in recent years. Fox (U.S.A.) discussed the general concept of Galerkin (spectral) methods. He indicated that as we begin to encounter increasingly complex situations for which air quality models are required, we must turn progressively toward the fundamentals. In the case of air quality these are the complete set of partial differential equations which describe the motion of the atmosphere, coupled with the transport and transformation of pollutant species. This set also must include some closure mechanism to relate the Reynolds stresses and turbulent fluxes to the mean values of velocity and concentration. These nonlinear partial differential equations must then be solved. The computer, of course, allows us to consider such complex systems, although the problems of solving nonlinear partial differential equations are considerable (Fox, D.G. and Deardorff, J.W., Computer Simulation of Multidimensional, Nonlinear, Subsonic, Incompressible Flows, J. Heat Transfer, Trans. of ASME, Nov 1972, 337-346. Two general approaches exist, namely, by approximating the continuous variables over a discrete grid, generally known as finite-differencing, and secondly by expansion of the dependence of the solution on one or more of the independent variables into a series of smooth functions, that are usually orthogonal. The latter is generally known as a spectral (Galerkin) technique. Many of the errors of approximation which can create great difficulties when applying finite difference techniques can be removed by spectral methods.

Velds (Netherlands) referred to a publication of F. H. Schmidt ("An analysis of dust measurements in three cities in the Netherlands" Mededelingen en Verhandelingen 86 (1964) K.N.M.I.,De Bilt) who has analyzed two years of hourly dust measurements in the city of Rotterdam. A harmonic analysis, up to the sixth harmonic, of the diurnal variation in dust content clearly distinguished between the morning maximum due to human activities and due to the stability, which shifted through the year almost parallel with the moment of sunrise.

There was considerable discussion of the lognormal frequency distribution for pollution concentrations that had been mentioned by Busch in his opening remarks. Schneider (Netherlands) said that it seemed to him that, except for SO_2, the lognormal distribution was the exception rather than the rule. Olsson (Sweden) indicated that they had plotted frequency distributions by wind direction and found good lognormal distributions for some directions, but not for others. Weber (W. Germany) noted that the lognormal distribution appeared to fit well for long periods like a year, but not for short periods of a few months. Turner (U.S.A.) presented a summary of a paper on "Air Quality Frequency Distributions and Meteorology" that had been prepared as background material for the meeting by R. I. Larsen (see Chapter XV). This mentioned a number of statistical models. In general one should only expect lognormality for locations in typical city surroundings with a wide variety of surrounding sources. It was also mentioned that there may be departures from lognormality in many circumstances, although this may not always seriously affect the conclusions based on the assumption of a lognormal distribution. Gifford (U.S.A.) encouraged investigators to set aside a part of the data being used for the development of statistical models for testing the models with independent data.

Keddie (U.K.) said that much of the unexplained spatial variance in observed concentrations of pollutants is almost certainly due to small scale variations in the urban structure and source field and to "bad" or unrepresentative siting of the monitoring instruments. The BP Reading exercise found the best correlation between SO_2 concentrations and emissions was obtained by considering the emissions within 1-2 km radius of the monitoring site. Our analysis of data indicates that smoke concentrations are best correlated with emissions within 1/2 - 1 km radius. These figures appear to represent typical urban scales for sulphur dioxide and smoke emissions.

Although the use of eigenvectors is a very attractive technique of handling air quality data, one would not expect it to work as well on such data as on, say, the spatial description of a meteorological parameter. The main reason for this is the very local nature of air quality in the sense that its spatial distribution is very dependent on the distribution of sources, at least in urban areas. A very dense network of monitoring stations would be required to provide the necessary data base for a detailed eigenvector description of the pollution field. Such a description would of course depend on the source configuration and like other regression type (non-source orientated) models, could not be used for long term planning purposes or in another geographical location.

Busch (Denmark) emphasized the importance of the development of objective forecast methods. These models, which are not at all source oriented and cannot, therefore, be used for control strategy purposes, could be of great value in connection with the planning of emergency actions for air pollution episodes. A good example was Dr. F.B. Smith's model for SO_2 concentrations in London and Manchester that had been discussed at the last meeting.

Fox (U.S.A.) suggested that perhaps a fourth type of statistical modeling should be considered, namely, stochastic-dynamic modeling of air quality. One desirable alternative to either the completely deterministic model or the totally statistical variety would involve a combination of these two in such a manner as to calculate a most probable concentration along with an indication of the variability inherent in this calculated value. This type of modeling has been pursued for large scale numerical weather prediction by Epstein [Epstein, E.S., Stochastic Dynamic Prediction, Tellus XXI (1969) 739-759] and Fleming [Fleming, R.J., On Stochastic Dynamic Prediction: I. The Energetics of Uncertainity and the Question of Closure, Mon. Weather Rev., 99, Nov. 1971, 851-872; II. Predictability and Utility, ibid, Dec. 1971, 927-950].

SOPHISTICATION VERSUS SIMPLICITY IN AIR QUALITY MODELING

This topic was introduced by Dr. F. A. Gifford (U.S.A.) who described some of the simple models that he and Dr. S. Hanna had developed at the Atmospheric Turbulence and Diffusion Laboratory of the U.S. National Oceanic and Atmospheric Administration (see Chapter XVI). Their involvement with urban diffusion modeling began in 1969, when they had been asked to calculate the potential atmospheric concentration of tritiated natural gas in the Los Angeles Basin, as part of the U.S.A.E.C.'s Project Plowshare. The simple area-source diffusion model that was proposed was $X = CQ/U$, where X is the concentration at a receptor, Q is the average area-source strength in the neighborhood of the receptor location and U is the mean transport wind speed. The proportionality constant C varies somewhat with atmospheric stability, but is influenced only secondarily by source-area size and configuration in this simple model. The model had been compared with a rather large body of air pollution data, and in many cases was found to give an even better agreement with observed data than more complex models. This was true even for a recent extension of the original model by Hanna, that included the effects of photochemical reactions.

Several participants raised questions concerning the determination of the parameter C in the simple model. In reply Gifford pointed out that various situations have occurred depending on the particular air pollution application. To estimate the urban area source concentration pattern, it is not necessary to know C. For time-varying air pollution measured at a point, such as that from traffic, the initial value of concentration can be used to estimate C. Olsson (Sweden) inquired whether, in such time-varying applications, C should not be varied to reflect time changes in stability. Gifford said that this had not been done in the comparisons presented, but agreed that the point should be studied. In the case of long-term average pollution the constant C has been evaluated both by means of air pollution data and from equation (3) (see Chapter XVI). For non-reactive pollutants such as particles, the results are as indicated in the text. For SO_2 there is indication of removal, in that the "observed" C from pollution is smaller than that calculated from equation (3). Values of C based on CO data on the other hand have seemed anomolously high. We attribute this tentatively to CO sampler location, at curbside on busy city streets for most of the data we have used so far.

Keddie (U.K.) agreed with Gifford that, in the present state of the art, simple type models work adequately in most urban areas. However, in the "regional" scale problem, for example, the simple model of Gifford and Hanna would not be adequate, particularly if there are pockets of urban and industrial development.

Velds (Netherlands) commented in response to a question raised by Gifford in his detailed paper (Chapter XVI), regarding the correlation with $(\text{windspeed})^{-1}$, of daily SO_2 concentrations at 31 stations in the Rotterdam area. At the Royal Netherlands Meteorological Institute the SO_2 data had been correlated with a ventilation factor, expressed as the maximum mixing height divided by the mean windspeed in the mixing layer. This gave a very low correlation coefficient, which led them to the conclusion that mathematical models probably would not work during air pollution episodes. Furthermore, it is doubtful if Gifford's assumption that the average source strength was constant during that episode, holds true. During the episode an alert had been given whereby several SO_2 sources were closed down. Furthermore, the source strength is dependent on the height of the mixing layer, as there are SO_2 emissions at all levels ranging from 10 to 300 m altitude in the Rhinemond.

Fox (U.S.A.) agreed that the simple model was attractive, but noted that a single correlation statistic does not really evaluate the utility of the model. For certain cases the ATDL model might be appropriate, but for others it does not work very well. He referred to an analysis by McElroy, of the Meteorology Laboratory of the E.P.A., of Gifford's use of Veld's data and for which Gifford had obtained a very high correlation. By isolating the days with strong stable stratification McElroy was able to show a better correlation with mixing depth H than with $(\text{velocity})^{-1}$. Clarke, also of the Meteorology Laboratory, was pursuing this idea for an urban stagnation model which allows a transition from Q/U to Q/H when the stability becomes positive.

Olsson (Sweden) indicated that their studies had shown that wind speed, and then mixing depth, were primary variables in relation to air quality. Busch (Denmark) said that they had found good relationships between air quality and stability expressed by a bulk Richardson number.

Grønskei (Norway) said that it is important to analyze the purpose of the model consideration, in addition to the climate and topography, when making the simplifications of the actual processes for the model. In some areas simplified model calculations may satisfy most of the administrative needs. In other areas where, for example, systematic vertical motion often represents an important dilution process, this has to be included to make the model applicable.

Gifford (U.S.A.) expressed the opinion that the simple model would give comparisons with the pollution data for Cologne, presented during an earlier session, of a quality similar to that for the other cities as summarized, in his Table 1 (Chapter XVI), and offered to make the calculations. Turner (U.S.A.) mentioned a systematic comparison, by GEOMET Inc. of Rockville, Md., U.S.A., of a detailed model based on the Gaussian assumption, with several versions based on equation (3), for New York City. The results were generally consistent with those presented in Gifford's Table 1.

Olsson (Sweden) said that we should primarily strive for a physically sound model, but that the degree of "sophistication" or "simplicity" should be guided by the users' needs. To a large extent the degree of sophistication has to be dependent on the resolution of the available input data. Lack of accurate emission inventories as well as inabilities to correctly describe mesometeorological circulations and variations are of great concern. In general he believed that, from an applications point of view, they would like to simplify their models and were therefore looking with interest at the results of Gifford and Hanna. The latter are striking in some applications, and certainly contribute to our understanding of the modeling process. There are, however, most certainly applications for which a more complex model formulation is needed.

Fox (U.S.A.) agreed and said that he believed that the development of the capability of detailed meteorological models to specify wind fields on the urban and regional scales is necessary, and will result in improved pollution models. The hourly variations of the quality of the urban environment simply was a complex problem that required complex models. However, he stressed the need to separate the development of such models, essentially a research activity, from the pressures of operational air pollution activities.

Neumann (Isarel) said that at one of the previous sessions, comments were made on the low autocorrelation found in the concentration predictions of theoretical models for urban areas, as compared with the autocorrelation observed in measured concentrations. The models in question are steady-state models. He wished to point out that it may not be quite appropriate to compare predictions based on steady-state theoretical models with processes in cities. In cities the concentration of pollutants has a very pronounced diurnal variation, that is, we have a time-dependent process. Hence, in theoretical efforts the proper thing would be to make concentration predictions founded on time-dependent, rather than steady-state models. In a time-dependent model predictions for any given time depend on the initial conditions, and certainly on conditions predicted for earlier times. One can expect, therefore, a very much higher autocorrelation in the predicted concentrations for a time-dependent model than in those to be found in concentration forecasts by what one may call "independently" applied steady-state models.

CHAPTER V

Introductory Remarks to Workshop on Applications of Modeling and Users' Needs

Kay H. Jones
Environmental Protection Agency, U.S.A.

4th Meeting of NATO/CCMS Panel on Modeling
Oberursel, W. Germany: 28-30 May, 1973

INTRODUCTORY REMARKS TO WORKSHOP ON APPLICATIONS OF MODELING AND USERS' NEEDS

The CCMS was formally established in November, 1969, by the North Atlantic Council of NATO. It represents the mechanism whereby the member countries could extend their practices of the international transfer and application of technology to fields of environmental pollution - also to more general social problems that stem from technological development.

The goal is to show leadership in the solution of existing problems and to develope long-range goals to head off future problems that might be anticipated.

At the last meeting of this Panel in Paris, in October, 1972, Mr. McCormick, the former Chairman, gave a resumé on the background of the CCMS and the role of the Air Pollution Pilot Study. Mr. McCormick's paper was subsequently published in the "Proceedings of the Third Meeting of the Expert Panel on Air Pollution Modeling (#14)." I will not repeat all of that background, but would like to expand on his presentation and bring you up-to-date on the progress of the project. Then I would like to embark on the discussion for the 1st session of this conference which deals with modeler/user relationships.

Let me start off by stating that the Air Pollution Study was designed with one aim in mind, namely, to promote air quality management programs within the NATO member countries and others as well. To this end we have endeavored to demonstrate and document key elements that are a part of the systems approach to an effective management program.

The demonstration project was divided into two phases. Phase I was concerned with sulfur oxides and particulate pollutants; Phase II deals with hydrocarbons, carbon monoxide, oxidants, and nitrogen oxides, i.e., Phase I is primarily industry or stationary-source related and Phase II is mobile-source related.

Goals of the project include (1) an assessment of ambient levels of pollutants, an inventory of sources, and projected levels of air pollution in several major cities, (2) selection of appropriate air quality models that relate emissions to ambient levels, as well as assess and report on the current state of the art in modeling, (3) develop criteria documents that relate health and welfare effects to ambient concentrations, (4) develop control techniques documents that reflect the latest technology in this field, and (5) promote cooperation in research and development among member countries in the field of automotive low pollution power systems.

Initially, it was decided to conduct assessment studies in three cities: Ankara, Turkey; Frankfurt, Germany; and St. Louis, Missouri, U.S. Phase I and II studies have been completed for Ankara and St. Louis and reported on as appendices A and B, respectively, to the NATO/CCMS document "Guidelines to Assessment of Air Quality (#6)." Since that beginning, the interest of the international community has grown to the extent that there are now seven assessment studies either being planned, in progress, or completed. The Frankfurt report is scheduled for completion by Fall, 1973, and will appear as Appendix C. A study in Oslo relating primarily to SO_2 has been completed by the Institute for Air Research in Kjeller and published as Appendix D, and a follow-up study of CO impact is being contemplated. Other studies are underway in Rotterdam and Milan, and a study in Turin is in the planning stage. All of these assessment studies will be reported on as appendices upon their completion.

Development of criteria and control techniques documents are being carried out by two expert panels. These groups, made up of the most knowledgeable experts from the NATO and Non-NATO participating countries, meet to discuss and draft documents which are later published as official NATO/CCMS documents. To date, the Expert Panel on Air Quality Criteria has published documents on sulfur oxides (CCMS #7), particulate matter (CCMS #8), and carbon monoxide (CCMS #10). By mid-August the document on Nitrogen Oxides (CCMS #15) will be available, and by Fall of this year a document on hydrocarbons and photochemical oxidants will be published. This last document will complete the work of this panel, as it will have accomplished all of its original goals. The Expert Panel on Control Technology is finalizing work on control techniques documents for sulfur oxides (CCMS #12), particulate matter (CCMS #13), carbon monoxide (CCMS #18), hydrocarbons (CCMS #19), and nitrogen oxides (CCMS #20). These documents will be available by Fall 1973. Their publication will mean that this panel, also, has met all of the original objectives laid out for it.

In light of a recognized need for development of low pollution vehicles among the NATO allies, the United States, in November 1970, as part of the Air Pollution Pilot Study, introduced the Low Pollution Power Systems Development (LPPSD) Program. As a result of this initiative, a conference was called to discuss LPPSD the following February in Eindhoven, the Netherlands. At this conference a Memorandum of Understanding was circulated by the United States among the assembled nations. This proposed that multilateral agreement would become the framework for cooperation in LPPSD among auto-producing NATO countries in the future.

On November 14, 1972, at the CCMS Plenary meeting at NATO Headquarters in Brussels, six nations signed the Memorandum. These nations were: The United Kingdom, France, Italy, Germany, the Netherlands, and the United States. We are also seeking the cooperation of two non-member countries who have strong industrial interest in this field, namely, Japan and Sweden.

Provisions of the memorandum call for:

- Direct information exchange
- Technical symposia
- Collaborative projects

The U.S. input to the LPPSD information exchange will come from the Advanced Automotive Power System Program (AAPSP), which provides for Federally sponsored research and development to produce an unconventionally powered, low pollution automobile. In Germany the Ministry of Research and Technology supports research on gas turbines. In France the Institute for Transportation Research is investigating noise and pollution abatement from conventional engines. In the Netherlands the Stirling Cycle is of great interest. Additional industry research is being conducted on diesels, stratified charge, rotary engines, battery and other concepts, such as hybrid power plants. It is expected that industry, as well as governments, will play key roles in this information exchange.

A second LLPSD conference is scheduled for October 15 - 19 of this year, to be held in Ann Arbor, Michigan.

As you may recall, this modeling panel was established to advise on the modeling aspects of the assessment studies which have been undertaken as part of the pilot project, as well as to make technical appraisals of new research modeling techniques. This panel has become the most active international forum on this subject, and it is our sincere feeling that this aspect of the pilot study should be continued beyond the official termination of the air pollution pilot study, now scheduled for the Spring CCMS Plenary, 1974. In this regard the panel can take on a new role of bringing together the "model user," that is the "air quality manager," and the model developer. Models are now ready for applied use, and this new panel activity can undertake the demonstration of a wide variety of modeling techniques, which are now available to the "users" within the NATO community. Such activity will greatly enhance our confidence in the finite solution of air quality management problems, rather than having to rely on less precise judgmental solutions.

To launch this morning's session I would like to probe what I consider to be a key problem area in the modeler-user relationship. It is not my intention to promote a discussion of the needs of the user in terms of the problems he needs solved and where models might apply, because I think this has been adequately covered in previous forums of this panel, by Warren Johnson and others (see CCMS Document #14, Air Pollution Modeling). What I do want to pursue is the communications gap that exists between modelers and users. A few general examples of this problem which come to mind and reflect this gap are:

(i) Many modelers wish to look upon their work as a continuing scientific research endeavor, rather than developing a dynamic tool for application in air quality management programs. Because of the copious number of caveats and qualifications, rather than confidence limits, that the modelers place on their results, the users tend to mistrust the output as being more of a black art rather than engineering.

(ii) The antithesis of (i) often occurs when users employ the results without the confidence limits to reach very tenuous decisions. In my opinion the modeler must be relied upon to describe the confidence limits of his results in as explicit a fashion as possible.

(iii) Users at the policy decision level normally do not have the slightest working knowledge of modeling, and hence lack confidence in the output product when arguing in the political arena. This is particularly true in the short- and long-range environmental management planning field where, in my opinion, models can make their biggest contributions in projecting air quality impact.

(iv) Air pollution modelers should make inputs in the data analysis for all types of air quality modeling, even through the meteorological factors are not explicit variables in the model, e.g., roll back modeling. All too often their inputs are not sought or rendered.

(v) Users have little appreciation for the research costs for improving the atmospheric modeling science, possibly because the modeler does not convey a cost-benefit analysis regarding his proposed work to the user, in this case the R/D manager. Users generally do not want to invest in research which does not have a time boundary for completion.

These examples are not meant to be inclusive or mutually exclusive, but to illustrate some of the deficiences I have observed over the past few years. In my opinion better communications between modelers and users is a must if the gap is to be closed rather than widened.

I firmly believe that this panel can undertake an activity to help solve the above cited problem by focusing some of its future effort, e.g., devoting at least one day of future panel meetings, to a joint modeler/user program I have not formulated an explicit plan but I would like to bring some key users to this forum, where we can play air quality games using the various "proven" models at hand and where (1) we instill confidence in the users concerning modeling, and (2) at the same time have the users come to understand the modeling science and the problems associated with improving it.

With this brief introduction, I would like to open up the floor to discussion, and hopefully by lunch we will have roughed out a program for the marriage of the user and the modeler.

Chapter VI

Introductory Remarks to the Workshop Session on "Validation of Air Quality Simulation Models"

4th Meeting of NATO/CCM Panel on Modeling

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Free University of Berlin

In order to avoid the impression that mathematical modeling of air pollution is only an intellectual game, measurements must be made and field experiments conducted to validate the models. At an early stage of the Bremen modeling effort the requirements of validation of the model were imposed by the people who provided the financial support for modeling. It will be best to describe the procedure by which we did this. The model developed for Bremen is a statistical model which produces all possible concentration fields, not in the sense of time series, but as an ensemble of such fields. At each grid-point in the city, and for a given period of time, an ensemble of concentration values is produced from which statistics can be derived. For example mean values or percentiles can be obtained. Plotting such parameters of the ensemble provides information which has a very high value for many planning purposes. On the other hand such information also allows monitoring stations for validation of the model to be placed at strategic locations, and determination of the minimum number for a satisfactory description of the structure of the field. The model can also interpolate between the monitoring stations.

Having these plots we were able to design a monitoring network for model validation in the following way. An isoline of mean value was first chosen on which stations were located to represent the structure of the field. These locations were chosen, however, so that they were not especially favourable for the simulation with the model. For example, one station was located near an industrial plant where there was inadequate information about the low level emissions. Another station was located so that it was separated from the center of the city by a large park. A third station was surrounded by a large water area although located in the very center of the city. Then a heating period was chosen (1967/68) in which half-hourly mean values of concentrations were available by measurements and also by simulation computations. A first look showed that the agreement between the two time series was rather poor. However, both ensembles were then formed and the statistics of these ensembles were compared with each other. The agreement between measured and simulated statistical parameters was quite good for two stations. The disagreement at the other station showed clearly that the source inventory near the industrial plant in fact was incorrect. After a correction of the inventory the agreement became satisfactory.

The most critical test for validation of the model is performed when statistics are compared for each wind direction separately. In this way we obtained SO_2 wind roses of the mean value and the percentiles. This is a much more detailed validation technique for the model, and if good agreement is obtained in this case then the model can be considered as a good one for the purposes for which it was developed. It is natural that the differences in this test are larger than for the case without separation of wind directions. However, the differences in the case of Bremen were comparatively small. On the other hand a disagreement between measured and simulated SO_2 wind roses clearly shows the input of pollutants from other regions. This was demonstrated when air pollution climatology of the city of Dusseldorf was simulated. In Dusseldorf almost 50% of the load is due to transport from other regions. I would suggest testing climatological models of urban air pollution by means of such wind roses.

It should be mentioned that the simulation does not provide a concentration value exactly at that point at which the monitoring station is located. Instead we calculate concentrations values at 25 grid points within a 500 by 500 meter area around the station and then apply an averaging operator to these calculated values. The average was considered to be the representative concentration value for the location of the station.

With regard to the validation of time-dependent models, I believe that this will be a much more complicated task. The simulation with the time-dependent model suffers from a lack of knowledge of the initial conditions. It must be shown that this lack of knowledge does not affect the predicted concentration values. In principle it is almost impossible to measure the 3-dimensional fields of initial concentrations. From an initial condition distribution the deterministic prediction then produces a probability distribution of the future state. It might be possible that inaccuracies in the initial fields could be shown to be important or not important for the predicted state. In general a stochastic forecast of concentration fields will be preferable, not only because of the lack of initial conditions, but also because of an inadequate knowledge of the physical processes involved and of the meteorological parameters that must be used in the model. In this way one will get values for mathematical expectation and standard deviations from the expected value.

Summary

Up to now we are able to validate climatological models of air pollution by means of a comparatively small number of monitoring stations. The preferred method of testing the model is by the use of concentration wind roses. Validation of time dependent models should take into account the stochastic nature of the prediction and should use modern concepts of space and time sampling theory.

Chapter VII

Introductory Remarks to the Workshop Session on The Role of Regional Air Pollution Studies in Model Development

4th Meeting of NATO/CCMS Panel on Modeling

W. Klug, Technische Hochschule Darmstadt

Chapter VII

INTRODUCTORY REMARKS TO THE WORKSHOP SESSION ON "THE ROLE OF REGIONAL AIR POLLUTION STUDIES IN MODEL DEVELOPMENT"

4th Meeting of NATO/CCMS Panel on Modeling

W. Klug, Technische Hochschule Darmstadt

When I was first asked to make some introductory remarks at this workshop session, I became aware of the fact that I had always thought of the role of Regional Air Pollution Studies in connection with model development as being related primarily to the validation of the models. But this was obviously not what the organizers of the meeting had in mind when they chose this topic, because there was already a workshop session devoted to the validation problem. So I had to try to discuss what other possible roles these studies might have.

Before we start the discussion on the topic of this session let us consider what we mean by the term "Regional Air Pollution Study." As you will probably all know, the term has been used before (for example in connection with the St. Louis Study or with the "Untermain" investigation) and in order to open up the discussion I would like to state what in my opinion are the minimum requirements for a Regional Air Pollution Study. The following information should be available in an area of minimum size of about 30 x 30 km^2 with known topographic features:

(1) Concentration measurements of one or more constituents (SO_2, NO_x, CO_x, . . .) with a density of the order of 1 per 25 km^2 to 1 per 100 km^2, obtained either continuously or discontinuously.

(2) Source inventory estimates, which contains detailed information about large sources (like power stations) and less detailed about smaller sources (like domestic heating). Time variations in source strengths must be included.

(3) Meteorological data, where as a minimum the following data should be available: the horizontal wind field near the surface, surface temperature, temperature gradient in the lowest 500-800m above the surface. It would also be desirable to have full synoptic observations, information on turbulence characteristics, etc.

(4) The data mentioned under (1) and (3) should be available not only in form of statistics but as synoptic (synchronous) distributions.

(5) The data must be obtained for a period of at least one year, preferably for a number of years.

Assuming now that a regional air pollution study in the above detail is available, what conclusions can we draw from the evaluated data for the development of models? Possible conclusions might be:

(1) From the structure of the concentration field one can infer how detailed the model calculations would have to be in order to represent relevant features of this field, i.e. the necessary minimum grid size.

(2) From the concentration data in connection with the synchronous meteorological data, deductions can be made concerning the type of model that has to be used. For instance if it were found that

appreciable concentrations occurred only under very light wind conditions with varying wind directions, we could be reasonably sure that a Gaussian plume model would not be appropriate.

(3) From the structure of the concentration field under different meteorological conditions it might also be possible to obtain estimates of the relative contributions of different types of sources. This could also be inferred by considering ratios of concentrations of different constituents.

(4) From the study it should be possible to infer whether or not sources outside the area under consideration have to be taken into account under certain meteorological conditions.

Finally let me make one suggestion: in the present stage of knowledge I would suggest that all regional air pollution studies should be accompanied by a simultaneous model development program. The relatively small effort (and money) compared to the total would help to improve the models, so that in the long run model calculations could largely take over the role of dense concentration networks, although -of course- without replacing the need for all measurements. These relatively few measurements could then be taken at strategically important points.

The ensuing discussion started with a description of the Environmental Protection Agency - Regional Air Pollution Study at St. Louis, Miss. In this connection the panel rather unanimously made a suggestion to the U.S. EPA, that the St. Louis data should be made available to all "model builders" as a basis for validation of models. After some other reports on regional studies by the British and Swedish observers at the meeting, the discussion focussed on the definition of the word "regional." After considerable discussion it was clear that a unique definition could not be given. Several suggestions made were:

(1) a definition based on characteristic times and horizontal distances of the order of 10 hrs. and 100 km.

(2) a geographic definition, where we include more than one city in the same general neighborhood.

(3) a definition based on a distance scale over which the concentration correlations exhibit a marked decrease, i.e. 30-300 km.

(4) a scale such that other meteorological processes have to be included in the modeling (e.g. scavenging processes, absorption at the ground, etc.)

(5) a political definition, by which an area is defined which has common political interests.

Although the above only indicates some examples of the interesting ideas that were put forward, they are typical. Finally, it was concluded that the main role of regional air pollution studies is to provide relevant data for model development and validation.

Chapter VIII

Introductory Remarks to the Workshop Session on "The Role of Empirical/Statistical Modeling of Air Quality"

4th Meeting of NATO/CCMS Panel on Modeling

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It may be appropriate to start with a reference to a letter that I received from Mr. K. L. Calder in March 1973, and in which he asked me to lead the discussion of this workshop. In this letter he says, "It was felt that the topic "The role of empirical/statistical modeling of air quality" might be an appropriate one for discussion at this time, since with one significant exception (Barrie Smith's paper on SO_2 prediction for London and Manchester that was presented by Frank Pasquill at our last meeting) the topic has been almost entirely neglected in our discussions to date. Perhaps one reason for this state of affairs has been the historical belief that air quality models based on statistical regression type of analysis are not source-oriented and therefore are largely useless for control strategy analysis in terms of the contribution of individual sources to the degradation of air quality. Also, of course, is the feeling that insofar as the statistical models are empirically established they will be specifically restricted in application, e.g., as regards geographical location, meteorological regimes, etc. Although this may be the case I am unaware that it has been clearly demonstrated that these limitations are really inherent in all statistical-type of air quality modeling. The question may be asked as to whether, with an appropriate analysis, a source-oriented statistical-type of air quality model could be developed which did not involve prior specification of meteorological dispersion functions per se and incorporation of these as in present air quality models. My thought here is that for given "meteorological conditions" these dispersion functions play the role of transfer functions between the air quality distribution and the distribution of pollutant emissions, and if one were smart enough might therefore conceivably be obtained empirically by a mathematical inversion technique (as, for example, by numerical solution of sets of integral equations) utilizing accumulated data on the distributions of air quality and emissions. If this could be accomplished then maybe a major shortcoming of the current statistical models could be removed and we should then in effect have an alternative to the customary meteorological-dispersion type of modeling. I mention all this because I think it is an important question that should be resolved one way or the other. What do you think?" In terms of a general function - theoretic approach to the problem that I have very briefly outlined on the blackboard, it seems that it may be possible to develop such a source-oriented approach as Calder has in mind, although this may require a number of special simplifying assumptions.

In opening up the discussion of this workshop and to avoid unnecessary arguments about the definition of empirical/statistical models, I would like to suggest that we adopt an ad hoc approach and consider three different types of statistical schemes that are currently being used in air pollution investigations. Statistical schemes can be used in two different ways, namely, in either an analytical or in a predictive fashion. They may be source-oriented to various degrees. The three types that I would like to propose for consideration are:

1. The purely statistical approach in which one tries to make predictions without directly using, or without having any knowledge of, the physics of the problem. An example of such a model is the assumption that the logarithm of the concentration is Gaussian process which, with additional assumptions concerning the auto-correlation function, then makes it possible to make predictions concerning the statistical variation of concentration when a different averaging time is used.

2. The traditional objective forecast method, in which some kind of reasonable expression is developed on the basis of experience and physical arguments, and which contains parameters that are then determined by some best-fit procedure utilizing the existing data.

3. An analysis by use of empirical-orthogonal functions. This method is based on expansion of the pollution fields in a series of orthogonal functions that are determined in such a way that the series converges as rapidly as possible. It appears to be a powerful tool in the analysis of the spatial variation of air pollution concentration. However, many problems remain to be solved before one can ascertain the practical usefulness of this approach.

Chapter IX

Introductory Remarks to the Workshop Session on "Simplicity Versus Sophistication in Air Quality Modeling"

4th Meeting of NATO/CCMS Panel on Modeling

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Simple urban air pollution models are not necessarily unsophisticated. A simple area source diffusion model has been developed and extensively tested at ATDL, Oak Ridge over the past three years. The bases for this model are the observations that: 1) concentrations at a receptor point can only be influenced by sources in a narrow, plume-shaped upwind sector; and, 2) the grid scale of urban area source-inventory patterns are typically much larger than point-source plume widths. Consequently, only upwind variation of source-strengths and along-wind variation of diffusivity need be incorporated in an area source model.

An area-source model results from introducing these simplifications into a general area-source diffusion formulation such as Calder's, or that written out by Busch during this morning's session. This simple model has the following properties. Area-source concentration at a receptor point is found to be directly proportional to the average source strength and inversely proportional to transport by the mean wind. The proportionality parameter varies somewhat with atmospheric stability conditions but is influenced only secondarily by source-area size and configuration, in this simple model.

Urban air concentration values derived from this simple model have been compared with a rather large mass of air pollution data, as well as with values given by a number of more complex air pollution models. These comparisons include annual particle pollution mean values, annual and seasonal SO_2 and particle urban area pollution patterns (i.e., spatial distribution), short-term area pollution patterns down to one hour, time-varying CO (traffic) pollution values up to 48 hours, and photochemical pollutants.

Examination of a table of correlations expressing these comparisons shows that the simple ATDL model in all cases compares favorably with more complex models. In most cases the simple model in fact achieves a somewhat better correlation with air pollution data. The reasons for this can only be conjectured, although the result may be somewhat surprising in view of the great amount of detail that apparently is included in complex models. It seems from our experience with the simple model that the gross influence of variations of source strength, mean wind transport, and atmospheric stability exert the primary control over urban air pollution and must be accounted for first; and only then other factors.

Chapter X

Cologne Emissions Inventory

A status report on the Cologne pilot scheme for establishing an inventory of atmospheric pollutants.

Edited by the Minister of Labour, Health and Social Affairs, of North Rhine-Westphalia, 1972.

Notice for the reader

This is the English version of the complete German text contained in the original "yellow book" edited in late 1972 by the Minister of Labour, Health and Social Affairs of North Rhine-Westphalia under the title

"Emissionskataster Köln".

It does not reproduce the many maps, tables and graphs contained in the "yellow book" but will facilitate their study and interpretation as the paragraphs of this English version are in full correspondence with the German text of the original document.

Translation by

Dr. Egon Keller and
Anthony Seymour, B.Sc.

INTRODUCTION

At my request, the Rhineland Technical Supervisory Association and the Board of trade have collaborated closely since 1969 to compile an inventory of substances polluting the air of the Cologne area. The inventory covers pollution from domestic heating, vehicles, and industrial sources.
Industry has collaborated most commendably by providing information for expert assessment, and today writing up the inventory is an accepted routine. Extension of the inventory to cover the Ruhr area, as foreseen in the "North Rhine-Westphalia Programme 1975", will start at the beginning of 1973, when the investigations in Cologne are complete.

The Cologne inventory, regarded as a pilot scheme, has been a success, and the aim of this report is to provide a brief survey of our experience up to the present time. I hope it will lead to the introduction of similar schemes in all the Laender of the Federal Republic, because the more information we record the better the basis for a determined and forward-looking clean air policy.

Werner Figgen
(Minister of Labour, Health
and Social Affairs,
North Rhine-Westphalia)

Düsseldorf, December 1972.

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1. GENERAL

1.1

The emissions inventory; basis of a new clean air strategy.

1.1.1

Definition of an emissions inventory.

An area emissions inventory is a record of all sources of air pollution in that area, classified according to geographical position (Gauss-Krüger Coordinates)and the conditions affecting their emission (dimensions of the source; quantity and temperature of waste gases; nature and quantity of pollutant material; frequency and duration of emission).

There are point sources (for example, factory chimneys), line sources (for example columns of vehicles on roads), and area sources (of which a good example might be the chimneys of a residential area).

An electronic data-processing system is required for the proper storage of the data. Details of how to draw up an emissions inventory and how to use it have already been published (2).

1.1.2

Drawing up an emissions inventory.

When starting to compile an inventory, the sources to be considered are industry, domestic heating, minor industry, and traffic. Various methods are used. In industry, the variety of different sources and the large number of pollutant chemicals make it necessary to employ experts to investigate each individual plant. For domestic heating and traffic an overall approach generelly suffices.

In industry, the enquiry begins at the plant from which the emission originates. All emissions from the plant are taken into account, including those form clearly defined sources and those from diffuse sources, and without regard to whether they are of such a nature - or are present in such quantity - as to contribute to pollution of the atmosphere. Whether a particular constituent is of significance as an atmospheric pollutant in a particular area becomes clear later when the inventory is assessed. The essential data relate to sources, plants, and emissions. They are entered on the cards shown below, which display the entire spectrum of information (2).

The enquiry is carried out by technical experts who collaborate with plant management and enter their findings on the cards. The methods used for the determination of the quantities of material and the concentration of emissions range from rough assessment to selective measurement. In industry the inventory should be kept up to date mainly with data supplied by plant management under the terms of paragraph 16 of the Factories act, or obtained by technical experts when they return for later inspections. The draft of the Federal Immissions Protection Act (BT Drucksache VI/2868) provides that the Manager of a plant which requires approval shall provide an annual declaration of emissions (paragraph 25), which is to be entered in the Emissions Inventory (paragraph 38).

There is no doubt that the majority of emissions from domestic heating and small-scale industry result from combustion. The nature of the emissions and the amount - per unit area - can be determined by an overall approach. However, emissions from small business which do not result from combustion must be determined individually, as is the case in industry.

Nevertheless, the procedure can be greatly simplified on the basis of experience. To determine the emissions from combustion in domestic fires and small business, the first step is to ascertain the quantities of the various fuels used. When this has been done, specific emission factors are used to determine the emitted quantities (per unit area) of the relevant constituents. The fuel consumption per unit area, and the heights of the chimneys, are obtained from the records which the district chief sweep is legally obliged to keep. Officially recorded data are not sufficient to ascertain the total quantity of fuel per unit area, subdivided into coal, lignite, oil, and gas. Difficulties commonly arise, particularly in the case of apartments heated by a single stove, and these can only be overcome by sample enquiries. Here again the district chief sweep can give valuable help.

Investigations of emissions from traffic can generally be restricted to road traffic. Emissions per unit area are most easily determined as a function of the quantity of fuel consumed. Fuel consumption per unit area per unit time depends on the number of vehicles, their engine capacity or load category, and the operating pattern. Records of numbers of vehicles are obtained by counting at particular points, or from aerial photographs taken at various times. Operating patterns are studied by the use of test vehicles, fitted with recording equipment, which are driven through the area under study in all typical traffic situations. If the operating patterns are classified in categories, and if these are simulated on engine test benches or on roller test beds with representative vehicles, it is possible to determine the emission factors of the various exhaust gas constituents as a function of the pattern of operation. The emissions per hour per unit area can be determined from the number of vehicles per hour, using the emission factors.

After mechanical processing, data on domestic heating, small-business and traffic are recorded in the same way as data from industry.

1.1.3

Evaluation of the emissions inventory.

An area inventory of the kind described provides the necessary basis for detailed local statements and for more general statements on clean air policy at the supra - regional level.

1.1.3.1

For given zones within the area under investigation the emissions inventory provides an overall view of the contribution of individual emission sources or groups of sources to the total emission of particular constituents. The diffusion calculation makes it possible to work out the degree of pollution by a given constituent at particular points in the area.

1.1.3.2

Consideration of the relative proportions of individual constituents of immission leads to local and supra-regional conclusions regarding necessary improvements and precautionary programs. Diffusion calculations show the sources or groups of sources on which an improvement order will have the most lasting effect. If the costs of improvements and the advantages to man and the environment are taken into account, the emissions inventory can serve as the starting point for cost-benefit analyses. If the inventory showed that a particular type of pollution source is of predominant importance in densely populated areas, changes in the law could follow.

1.1.3.3

When there is a sudden, unexpected build-up of pollution, giving rise to public anxiety or to damage, meteorological data and dispersal calculations can be used to determine which of the listed sources is responsible.

1.1.3.4

In the approval procedure under paragraph 16 of the Factories Act the inventory of existing sources is considered in conjunction with the inventory of proposed new sources submitted for approval, and the dispersion calculation then shows the pollution which would result from the new plants at any chosen point in the affected area. It is also possible to calculate what improvements are needed in existing plants to ensure that the construction of new plants does not bring the total pollution above the accepted limit.

1.1.3.5

In city and regional planning the emissions list, together with dispersal calculations, serves to determine the necessary distance between existing residential areas and new industrial areas, or vice-versa, depending on the emissions from the industry. When assigning an area for industrial use, the existing or simulated inventories would have to be transplanted for siting.

1.1.3.6

The emissions inventory provides pointers as to which constituents of an emission are relevant from the standpoint of pollution. Dispersal calculations are easier and more reliable when particular points are established for the taking of measurements. The chosen points are those at which the highest concentrations of the particular emission constituent are expected, and this technique avoids the expensive measurement on an area basis by "the rule of thumb".

1.2

Preliminary comments on the Report.

The emissions inventory of the Cologne area is not yet complete. This is therefore a provisional report, from which final conclusions must be drawn with reservation. It is essential to be cautious when attempting to generalise on the basis of an investigation restricted to the particular industrial and economic conditions of Cologne.

The report is based on the results available up to the end of 1971. Corrections to the inventory which may be necessary from time to time as a result of changes in population density, traffic conditions, or industrial emissions - particularly those resulting from abatement measures - will not be made until the main investigation is complete. The data from the 1969 - 1971 investigation are thus not to be taken as absolute, but they do reliably indicate the order of magnitude of the emissions which were measured. Conclusions based on the emissions and pollution levels set out in this report - and particularly conclusions relating to specific areas - are only possible to a limited extent. For exact up-to-date information, it is always necessary to consult the current inventory.

The interpretations and evaluations of data which follow in a later part of the report are given only by way of example. The object of the report is to outline briefly the possibilities presented by the emissions inventory in improving the quality of the air in a region. It is impossible, within the framework of this report, to present all the evaluation programmes.

By use of the inventory in the ways described in 1.1.3, definite knowledge has already been gained which would otherwise have remained unproved professional conjecture.

Data on the relative contributions of different groups of sources to air pollution in the Federal Republic show considerable variation.
According to a report from the General German Automobile Club (ADAC) 47.2 million individual heating systems are responsible for 25% of the total emission of harmful waste gases. The Federal Centre for Political Education in Bonn, on the other hand, attributes barely 6% of pollutant emissions to domestic heating. According to the ADAC the other sources of such emissions are road traffic (40%) and industry (35%). The Federal Centre for Political Education attributes 60% to road traffic, 18% to industry, 13% to power stations, and 3% to burning of refuse.

The first point to be made here is that like is not being compared with like: 'what are harmful waste gases?' While waste gases from combustion processes in industry, domestic heating, and traffic comprise about ten constituents and are roughly comparable, industry - as the Cologne emissions inventory has shown - produces more than three hundred different air pollutants which do not feature in waste gases from domestic heating and traffic. If comparisons of air pollution are to be made, the constituents in question must be named. The Cologne study has also revealed that the relative contributions of different sources to air pollution differ to a great extent according to whether one considers the emissions or the resulting pollution. In this context the height above ground of emission has a marked influence on the amount of pollution in the immediate surroundings - and both domestic heating and traffic emit close to ground level. Industrialists long considered that industrial emissions produce relatively less pollution in the immediate surroundings because the waste gases are expelled through high chimneys. In Cologne this has proved to be not entirely true: from information available at the present stage of the investigation, it is, for example, clear that 45% of organic gases and vapours from industrial plants are emitted from sources below the ten metre level, and 84% from sources below the twenty metre level.
It follows that problems resulting from emission close to ground level are not restricted to domestic heating and traffic, but

can also be important in industry. A further point is that in industry, unlike domestic heating and traffic, a considerable proportion of the emission is not from clearly defined sources such as chimneys, but to a considerable extent from diffuse sources at a number of points on the site.
Thus, in the area under unvestigation, 37% of industrial emissions of organic gases and vapours from diffuse sources, for example pump and flange leakages, filling losses during the handling of mineral oil, and evaporation losses from tanks of mineral oil and mineral oil products.

Another important factor in comparisons of emissions and their relative contribution to pollution is the timing of the observations. In the summer months, for example, there are practically no emissions from domestic heating. Again, at night time, there is a significant reduction of emission from domestic heating and traffic, unlike certain emissions from continuous industrial operations. Finally, in an analysis of the relative contributions of different groups of sources, the locality under consideration must be exactly defined. Test calculations in Cologne have shown that conditions in the inner city, where there is considerable emission from domestic heating and traffic, are different from those on the fringes of the city, where there is a concentration of industry, but few dwellings and little traffic. Chiefly, the investigations have shown that carbon monoxide, nitrogen oxide, and hydrocarbon pollution from vehicle exhaust fumes in the streets of the inner city during the day is 5 - lootimes greater than that above the level of the buildings flanking the streets. This indicates that, in the traffic zones of the inner city, vehicles are the predominant source of waste gases prejudicial to health, and underlines the need for a drastic reduction of carbon monoxide, nitrogen oxides, and hydrocarbons in exhaust fumes.

In addition, the Cologne emissions list has pointed the way to new methods of assessment under the administrative approval procedure, and in urban planning. In a number of instances, the pollution to be expected as a result of setting up a particular plant has been forecast at the approval stage, which had never been done previously. Forecasts of this sort will be routine in the future.

The list is also used in calculating the appropriate distance between industrial and residential areas.

When a network of automatic pollution monitoring stations is installed in the coming years, the emissions inventory will provide valuable indications as to which constituents of pollution are to be covered, and where the stations should be sited for optimum performance.

This report does not reach any final conclusions as to concrete programmes of improvement in the Cologne area, but this most certainly does not mean that there has been no tangible achievement. To set up effective abatement programmes it is necessary first to complete the investigation over the entire area, and then to interpret the findings in a uniform manner. Preparations for this interpretation are already in hand, and the work will be done immediately after the investigation has been completed. Conclusions have already been reached at the factory inspectorate level, and the necessary ministerial steps taken. Faults in industrial plant, giving rise to harmful emissions, have been noted by the factory inspectorate, and followed up. In many cases, however, there was no need for the inspectorate to take any action, because the industries concerned made the necessary changes on their own initiative. Following the emissions inventory investigations there has been a considerable improvement in clean air technology in industry in the Cologne area, and also in certain branches of industry elsewhere. In Cologne there has been a reduction in certain industrial emissions and thus - taking an overall view - an improvement in the pollution situation.

1.3

Survey of the Cologne area.

1.3.1

General data on the area under investigation.

The area of the investigation is shown in Map 1. Going from North to South it includes parts of the Dormagen, Monheim, and Leverkusen communities, Cologne City, the Rodenkirchen and Wesseling communities, and parts of the Cologne district and of the city of Porz and the community of Niederkassel. The total area is 521 square kilometres. Table 1 summarises land use in the area.

The population (1.15o.ooo; Table 2) is relatively dense, and averages 2.2oo inhabitants per square kilometre.

Out of a total of 112.5oo buildings in the area under investigation, about 1o5.ooo are wholly or partly used as dwellings (Table 3). The counts of buildings and of apartments in the year 1968 show the number of apartments in the area under study, and the type of heating (Table 4). To a great extent the relative proportions of the different types of heating are in agreement with the Federal average.

In the area of the study there are about 5oo.ooo employees, of which 43% are engaged in industry (Table 5).

1.3.2

Weather conditions in the Cologne area.

The weather in the Cologne area between Wesseling and Dormagen is substantially affected by the broad valley of the Rhine between the Bergische Land area to the east and the foothills to the west. The wind most commonly blows down the valley. Wind statistics over a period of years, based on the records of the German Weather Service, show the prevailing wind at the Cologne-Bonn airport to the East-Southeast (125°). Figure 1 shows the relative frequencies of winds from different directions at the airport. The arrows point the direction in which the wind blows, and the length of an arrow indicates the percentage frequency of wind in that direction.

Table 2 shows the distribution of wind speeds in the Cologne area. The most common speed is 3 metres/second.

The turbulence of the atmosphere in the area under study is indicated by the frequency of the different levels of stability in Table 6, which is based on Klug's classification (3).

The weather of Cologne is further illustrated by the long-range average data in Table 7 (air temperature, precipitation, duration of sunshine, cloud, and the number of heating degree days for the individual months of the year).

2. EMISSIONS INVENTORY

2.1

Status of the investigations.

Map 2 summarises the status of the investigations on the 31st December 1971.

Of the industrial areas shown on the map, covering 29 km^2, a total of 45% was included in the study. By the 1st May 1972, investigations were almost complete in a further 17% of the industrial areas. About 35% of the industrial areas are not included in the study.

In respect of domestic heating and small business, 79% of the areas in question, totalling 155 km^2, are included in their entirety. About 60% of the road traffic area shown has been included. In the part of the city centre lying to the left of the Rhine particular care was taken to include industries from whose plants high proportions of organic emission were expected. These investigations are not yet complete. All furnaces and boilers in the entire area of Cologne city are included.

An overall appraisal of emissions and the resulting pollution in the area under study - which is to be regarded as a closed area of air pollution - will be possible only when the list is complete. For this reason we are presenting separately the results so far obtained for industry, domestic heating and small-scale industry, and road traffic.
Part 3 of this report, based on a sub-area, outlines the possibilities of a comparative approach. However, to give a preliminary review of the overall results, Figure 3 shows the proportions of carbon monoxide, sulphur oxides, nitrogen oxides, other inorganic gases, organic gases and vapours, and dust in the emissions from various groups of sources in the area which has been investigated up to the present time (Map 2).

For individually studied industrial plants, for industrial furnaces (studied on an overall basis), for road traffic, and for domestic heating and small-scale industry, it shows the relative proportions of the constituents of emission. In this presentation the sum total of the individual source groups is in every case taken to be 1oo%. Because not all aspects of the various investigations are equally far advanced, it was impossible to adopt a presentation in which the actual quantities are stated alongside the percentages of the emission constituents.

Consideration of the industrial emissions, determined by individual investigations, shows the importance of oxides of sulphur, which account for 43% of the total emission. Next come the organic gases and vapours, with 29%, and then the oxides of nitrogen (19%) and carbon monoxide (5%). Other inorganic gases and dusts account for a mere 2% each.

Industrial heating, which was investigated on the overall basis, as used for domestic heating and small business, emit 67% sulphur oxides, 17% nitrogen oxides, and 5% carbon monoxide. Organic gases and vapours here amount to less than 2%. Dust accounts for almost 9% of the total emissions of the industrial furnaces.

The most important emission constituent of traffic is carbon monoxide, accounting for 91% of the total. Oxides of nitrogen account for 4%, and oxides of sulphur 1%. Organic gases and vapours in the exhaust fumes total 3,5%. Dust amounts to only o,3 %.

In the domestic heating/small-business source group, carbon monoxide, with 73%, is again the most abundant constituent. Oxides of sulphur account for 12%, and oxides of nitrogen for 3%. Organic gases and vapours total 7%, and dust 5%.

2.2.

Emissions from industrial sources.

The assessment which follows covers 22 chemical firms, 8 petrochemical firms, and 14 other enterprises producing relevant emissions. Also included in the inventory were the boiler plants of a further 164 industrial firms.

The assessment takes into account data from about 575 large plants, and includes descriptions of the emissions from about 6.5oo individual plant units. These plants and their constituent parts release emissions into the air from about 1.8oo defined outlets. In the investigations of diffuse sources (for example leaks) about 7oo line and area sources werde defined.

The emissions inventory upon which the assessment was based includes about 61.5oo statements of information, about 5o.ooo of which relate specifically to emissions from the plants. These statements comprise a total of 1,5 million units of information.

2.2.1

Constituents of emission.

The emissions inventory provides information on 338 individual constituents or mixtures. In some cases where selective methods of determination were not available within the scope of the study, it was necessary to show the mixture as such. 26 inorganic and 2o8 organic constituents were determined as gaseous emissions. 1o4 constituents were dusts.

In table 8, which summarises the emissions from industry, some constituents which were determined individually have been grouped so as to achieve a clearer visual presentation. The details follow in Tables 9 to 25. Of the industrial emissions so far studied 7o% are inorganic gases,27% are organic gases and vapours, and dusts account for less than 3% of the total. The total of inorganic gaseous emissions is put at about 8o.ooo metric tons/year. The greater part (64%) is sulphur dioxide; oxides of nitrogen account for 26%. There is relatively little emission of carbon monoxide from industry, totalling only 6,4% of the total emission of inorganic gases. A further 3,4% are other inorganic gases, given in Table 9. These are for the most part hydrogen, ammonia, and hydrogen chloride. This report does not give full details of the individual constituents.

The emissions inventory puts the total quantity of organic gas and vapour emissions at 3o.ooo metric tons/year. Of this total, 68% are hydrocarbons, and 32% other organic gases and vapours, given in detail in Tables 1o to 21. In Table 1o the hydrocarbons are divided into various sub-groups, of which the aromatics (27,6%) account for the greatest part of the total. Next in order of quantity come the benzine hydrocarbons (23,6%) and the lower hydrocarbons (23,4%). The remaining 25,4% is divided into three further sub-groups, shown in Tables 11 to 14.
Of the aromatic, toluene, with 45%, is the most abundant, and the various xylenes (totalling 32,6%) are also important. Test benzine (9,8%) and benzol (8%) also occur.

Aromatics should also occur in the benzine hydrocarbons sub-group: in the framework of the investigations it was impossible to demonstrate them separately. The benzine hydrocarbons are shown subdivided into various fractions in Table 12. The most abundant are the low boiling fractions with boiling limits lying between 35 and 1oo° C. Hydrocarbons originating from special carburettor fuels are given separately. The lower hydrocarbon sub-group comprises ethylene (3o,8%), methane (18,5%), propane (11,5%), propylene (11,4%), and other lower hydrocarbons, listed individually in Table 13 (27,8%). Heavy hydrocarbons are given in detail in Table 14.

In the case of the hydrocarbons shown in summary form, it was impossible to go into greater detail because of the expense incurred in detailed measurements.

Tables 15 to 21 give details of the chlorinated hydrocarbons, epoxides, alcohols, esters, ketones, aldehydes, and other individually determined constituents. Again, this report does not list all the individual constituents which were determined.

88% of dust emissions (see Table 8) result from combustion processes. Other dusts are encountered only in small quantities. Heavy-metal dusts account for 2,8%. Tables 22 to 25 specify the individual dust constituents.

2.2.2

Emissions specific to particular branches of industry.

An absolute comparison of the emissions from various branches of industry would be pointless at the present stage of the investigations (see 2.1).
In the absence of such comparison, Table 4 gives the contributions of the emission constituents carbon monoxide, sulphur oxides, nitrogen oxides, other inorganic gases, organic gases and vapours, and dust, for various branches of industry, the overall total of these categories amounting to 1oo% in each case. The contributions of various constituents to the total emission of industrial furnaces - which were studied on an overall basis - is given separately, because up to the present time these furnaces have not been assigned to a special branch. In metal processing plants and chemical plants the proportion of sulphur oxide emissions is relatively low, while the proportions of organic constituents are relatively high. For 'other industrial plants' the level of nitrogen oxide emission is particularly high, because high performance gas furnaces are included. Tables 26 to 3o give specific emission data for the various branches of industry. It is clear that in all branches of industry the emissions comprise numerous different individual constituents, and as might be expected, the number of constituents is greatest in the case of the chemical industry.

2.2.3

Emissions specific to particular plants.

Table 31 reviews the contributions of different types fo plants to the total emission from industry. Furnaces emit 78,5% of the inorganic gases, 83,4% of the sulphur oxides, and 93% of the nitrogen oxides. On the other hand they emit very small proportions of carbon monoxide and other inorganic gases, which come mainly from chemical reaction plants, processing plants, and others.
Sulphur oxide emissions from furnaces were to a large extent calculated as sulphur dioxide from the proportion of sulphur introduced into the furnaces along with the fuel. The proportions of oxides of nitrogen emitted by furnaces were calculated by the use of emission factors deduced by Kolar (4) from American investigations. 2o% of the other inorganic emissions were calculated as leakage from seals using suitable emission factors (5-1o).

The proportions of the remaining inorganic gases were obtained to a large extent by measurement, and partly by comparison from the result of similar studies. More information on how the data were obtained can be had from Table 32.

Furnaces do not play an important role in the emission of organic gases and vapours. These are emitted mainly by processing plants, plants for the application of surface coatings, containers and storage sites, conveying and filling plants, chemical reaction plants, and other, unspecific plants. Emissions from leaks amount to 19,5%; these were determined by methods based on published work (5-1o). Emissions from containers and storage sites, and from filling plants, were to a large extent determined by calculation, on the assumption that the layer of gas above the container is practically saturated with the chemical in question. The filling rhythm of storage containers, and the quantities of chemical handled by filling plants were generally obtainable direct from the firm's records. In the case of plants for the application of surface coatings it was again possible to rely to a large extent on calculation, starting from the assumption that the solvents used in coating processes evaporate almost completely into the air. The extent to which this assumption was true was checked in each individual case. For further information see Table 32.

Table 32 shows, for the industrial group of sources, which emissions were determined by measurement and which by calculation or comparison. It can be seen that the emissions of inorganic gases, particularly oxides of sulphur and nitrogen, were largely obtained by calculation. By way of contrast, 79% of the carbon monoxide emitted was determined by measurement. Of the other inorganic emissions, whose contribution to the total of emissions is only small, a total of 37% was determined by measurement, 28% by calculation, and 35% by comparison with similar cases.

For organic gases and vapours, 49% of the quantity stated in the emissions list was demonstrated by measurement.+) A total of thirty-seven per cent of the quantities stated in the list (storage sites, filling plants, seals) was obtained by calculation, and 14% by comparison.

It must be emphasised at this point that there are individual cases where measurement is not possible with the equipment at present used in pollution control, or where it would involve considerably expense. This is a pressing problem, for example in the cases of flares, sewage filter beds, and the more exact determination of leakages.

+) 31% of which by selective methods.

2.2.4

Emissions specific to particular sources.

Table 33 shows at what heights above ground level the emissions are released, and for the most important constituents or groups of constituents the same information is also presented in the form of graphs (Figs 5 - 1o). Essentially, they point to two important conclusions:

1. Industrial emissions from furnaces, that is to say, particularly, sulphur oxides, nitrogen oxides, and light ashes, are mostly emitted at great heights.

2. Organic gases and vapours for the most part find their way into the atmosphere near the ground level - mostly at heights below 2o metres. This is why there are often unpleasant smells in the immediate vicinity of industrial enterprises whose plants emit organic gases and vapours.

Table 34 lists emissions from defined and from diffuse types of source.
Defined sources are devices whose sole purpose is the discharge of waste gases or waste air.

Among the defined sources a distinction must be drawn between those where there is unimpeded upward movement above the outlet, and those where upward movement of the gases is hindered. Diffuse sources comprise industrial equipment and apparatus from which emissions are released into the air in an uncontrolled fashion during normal working. Up to the present time, little attention has been given to diffuse sources within the framework of clean air schemes. It can be seen from the Table that 99% of inorganic gases reach the atmosphere by way of defined sources. This applies without restriction to emissions of carbon monoxide, sulphur oxides, and nitrogen oxides. Of the other inorganic gas emissions, about 3o% are from different sources.

To a large extent, these are the ones which are emitted close to the ground. 37% of organic gas and vapour emissions are from diffuse sources, and 63% from defined sources.

2.2.5

Rhythm of emission.

Emissions from industrial plants are not constant, but vary according to the condition of the plant and the throughput. These variations often depend on the rhythm of work in individual plants, and therefore show a time pattern. Figures 11 and 12 show the time pattern of industrial emissions. Figure 11 shows the pattern of emissions during the course of the day, based on the average over the year. The effect of plants working a single shift from 6.oo to 17.oo hours can be seen, and more particularly the effect of two-shift plants operating from 6.oo to 22.oo hours. Figure 12 shows in a similar way the pattern of emissions over the course of the year.

2.3

Emissions from domestic heating and small business.

In the area in which emissions from the above source group have so far been studied, there are approximately 913.ooo inhabitants, that is to say 79% of the total population of the area under investigation. It is in the study of these emissions that the greatest progress has been made.

Close on 3oo.ooo chimneys were included, mostly belonging to the heating systems of buildings. Table 35 shows the number of chimneys involved, classified according to the fuel used.

The heat generated by installations for the heating of buildings, and by the furnaces of small business, totals $1o \times 1o^{12}$ kilocalories per year. Of this, 98% goes into the heating of buildings, and the remaining 2% is generated by the furnaces of small business (Table 36). About 6o% of the heat comes from the combustion of light fuel oil. City gas and natural gas account for 1o%, and solid fuels for 3o%. The relatively high gas consumption of small business furnaces (72% of the heat demand) is striking. Absolute consumption figures for the various fuels are given in Table 36.

Tables 37 and 38 list the various types of installations covered, and their contribution to the total heat generated. A distinction is drawn between boiler installations for the heating of private households, business and office premises, buildings used for more than one purpose, schools, hospitals, and hot houses. In small business enterprises, furnaces are particularly to be found in bakeries, butchers' premises, laundries, and joinery workshops.

In the field of small business, installations other than boilers were included, in particular 227 chemical cleaning units with a total capacity of 4.3oo kilograms. Also included were 639 filling stations and other points of sale of petroleum products, with a total turnover of 41o.ooo.ooo litres/year. In butchers' premises ordinary furnaces and also smoke-curing rooms were investigated. The list includes entries for 2o8 coldcuring installations and 187 hotcuring installations. Their consumption of wood shavings and sawdust totals about 1.25o metric tons/year. Also included were 8 car body firms with painting facilities, 8 refuse incineration plants, and 3 coffee roasting plants.

2.3.1

Emissions.

The emissions from the described plants are given in Table 39. The total emission is about 72.ooo metric tons/year, of which 88,1% is anorganic gases, whereas only

6,6% is organic gases and vapours, and 5,3% light ash. Carbon monoxide, accounting for 83% of the total emission of inorganic gases, is one of the most important constituents. About 14% of the inorganic gas emissions are sulphur oxides, shown as SO_2 in the emissions list. Nitrogen oxides, shown as NO_2 in the emissions list, account for 3% of the inorganic gases. Hydrogen chloride emissions from refuse incineration plants are of no importance in an overall assessment of the region.

Of the organic gases, only about 60% of the emissions come from boilers, namely a fraction of the hydrocarbons and the aldehydes, which are here shown as formaldehyde. About 24% of the organic gases are benzine hydrocarbons from filling stations and other points of sale of petroleum products, and about 24% are perchlorethylene from dry cleaning establishments. The remaining 8% of the organic gases and vapours come from smokecuring rooms, painting works, and other installations which were investigated separately.

Table 46 lists the proportions of the individual constituants which were determined.

2.3.2

Height of emission above ground level, and rhythm of emission.

For an assessment of emissions from domestic heating and small business the height at which the emission is released is important. Table 41 lists the proportions of emission constituents emitted at various heights above ground. The results are also presented in graph form in Figures 13 - 17.

Emissions of the domestic heating/small business source group show a typical daily and seasonal rhythm, principally due to the mode of operation of installations for the heating of buildings. Figures 18 to 21 show the seasonal and daily rhythm of emission of carbon monoxide, sulphur oxides, nitrogen oxides, and organic gases and vapours. In each case the highest levels of emission are to be expected in January, the coldest month of the year. They are greatly reduced in the summer months. In the cold season there is a peak of sulphur oxide and nitrogen oxide emissions in the morning between 6.oo and 8.oo hours. This time - dependence is not clearly pronounced in the case of carbon monoxide, because coal-fired boilers burn better when working at full capacity than when damped down (Figure 18). The emission of organic gases and vapour, mainly from small business (particularly filling stations and dry cleaning establishments) remains relatively high in the summer months (Figure 21). The daily rhythm of emissions of organic gases and vapours reaches a maximum between 16.oo and 19.oo hours, because this is a time when filling stations are relatively busy, and when dry cleaning establishments regenerate.

2.3.3

Emission factors.

Emissions from combustion points were determined by calculation on an overall basis. The emission factors used were derived from the literature (11 - 17) and from the unpublished results of the North Rhine-Westphalian Centre for Immissions Abatement and Protection of the Soil, and of the Rhineland Technical Supervisory Association. They are given in Tables 42 and 43. These are average values based on the performance of the plants at different work loads. Thus, for example, according to Kolar (4), nitrogen oxide emissions from boilers and furnaces are exponentially related to the performance. Emissions of carbon monoxide, dust, and organic gases and vapours from solid fuel boilers and furnaces are to a high degree dependent on the quantity of fuel burnt, because these installations are generally regulated by cutting down the supply of air. In oil and gas-fired installations the phonomenon is less pronounced, because they are generally regulated by switching the burner on and off. The different types of regulation were borne in mind in deciding on the emission factors. Table 44 shows the proportions of the emissions from the various fuels.

2.4

Emissions from road traffic.

2.4.1

Emission factors.

Many studies were carried out on a roller test bed to obtain the emission factors for road traffic. The test vehicles were so chosen that the emission factors obtained may be taken to be representative of road traffic. At the outset a distinction was made between cars and trucks, and between Otto engines and Diesel engines. Also, the dependence of emissions on the capacity of the motor and its age were taken into account. Information on these points was obtained from the registration statistics of the Federal Office for Powered Vehicles. Figures 22 and 23, based on these statistics, show the breakdown of cars and trucks into various categories of capacity. Most cars, for example, are in the 1ooo - 12oo cm^3range. About 93% of trucks are of engine capacities up to 6ooo ccs. Figures 24 and 25 show the breakdown of cars and trucks into categories of performance. According to these figures, over 78%of the cars are in the 3o - 59 horse power range, and they include 25% of the total of cars in the Federal Republic falling into the 4o - 49 horse power category. The power range of trucks is extremely wide, rising to 2oo horse power. Only 2,5% of vehicles are more high-powered than this. The breakdown of the cars and lorries by year of manufacture is given in Figures 26 and 27, which show that vehicles up to 5 years old are in the majority.

In order, to ensure that the subdivision of the test vehicles according to the above characteristics matched as closely as possible the actual traffic on the roads, the test vehicles

were selected exclusively from the 3o most commonly occuring types (representing about 2/3 of the total of cars). The number of a given type was based on the numerical proportion of that type in the Federal Republic.
Because of the low proportion of trucks in the traffic of big cities, truck emissions were determined from the test bed performance of only a few vehicles. Because there are so few trucks, the resulting limitation on the accuracy of the results has little effect on overall result of the emissions study.

To determine the emissions of the relevant exhaust gas constituents, test cycles were developed which closely correspond to actual traffic conditions. The test cycles comprise successive phases: idling - acceleration - constant speed - deceleration - idling. The time ratios of the individual phases, the average speed, and the average acceleration and deceleration in the test cycles correspond to those recorded by a test vehicle in road traffic. A limited number of test cycles at defined average speeds were chosen as being representative of all driving conditions in a given speed range. These representative driving conditions are also described as 'driving styles'. On the basis of their average speeds, driving styles can be arranged to correspond to particular traffic situations, as in Table 45.

The emission factors used in the emission studies (obtained from measurements on 44 cars and several trucks on the exhaust gas test bed) are given in Table 46 and 47. For one hour of driving time they give the specific emission values for carbon monoxide, nitrogen oxides, hydrocarbons, and oxides of sulphur in the case of petrol engines (cars) and also the specific emission of lead constituents, and for diesel engines (trucks) they give the emission of soot. The Tables also provide data on specific fuel consumption and the quantities of exhaust gas to be expected. With the help of these emission factors it is possible to calculate emissions on roads or on equivalent area sources, given the number of vehicles and the driving style.

2.4.2

Traffic levels.

The density of traffic in the area studied up to the present time was determined by traffic counts at various times of the day, and by examination of aerial photographs. At the same time the driving style was continuously recorded by a car fitted with a measuring device, which circulated with the traffic. Map 3 gives an overall view of the area which has so far been studied in respect of road traffic. By means of a coloured classification of the roads and of the areas which were studied on an overall basis, the map also includes a graphic presentation of the results of the traffic counts. The coloured lines and areas indicate the annual total of motoring activity. The overall results from traffic counts in the area so far studied are given in Tables 48 to 5o. For the different driving styles they give the annual total of motoring, the corresponding consumption of fuel, and the resulting quantities of exhaust gas. In all, they show motoring totalling approximately 79 million vehicle hours/year. More than 83% is accounted for by driving styles 3 and 4, that is to say city traffic in the speed range 22 to 55 kilometres/hour. Traffic on the 55 kilometre stretch of autobahn so far included in the study accounts for 5.5 million vehicle hours/year, i.e. 7% of the total. These figures indicate a total of about 2.8oo million kilometres/year. The corresponding fuel consumption is about 238 million kilograms/year, or 3oo million litres/year.
Out of the annual total of motoring, cars - with 73 million vehicle hours/year - account for 93%, and trucks only 7%.

Density of traffic, and style of driving, are particularly dependent on the time of day. By way of example, Figure 28 shows, for the area under investigation, the time pattern of traffic density and the relative proportions of the different styles of driving. Clearly, the peaks of traffic lie between

6.oo and 8.oo hours and 16.oo and 18.oo hours, and, equally clearly, these are the times when the proportion of slow-moving traffic is especially high.

2.4.3

Emissions.

With the help of emission factors (Tables 46 and 47) the emissions from traffic were calculated from the traffic data. For the sake of simplicity, motor cycle/side car combinations and small petrol driven vans were included with the cars. Because they were so few (3%), diesel powered cars were excluded.
Buses and relevant special vehicles were included with the trucks, and for the sake of simplicity it was assumed that they are all diesel-powered.

Figure 29 shows the time pattern of total emission over the course of the day. The relationship between traffic density (figure 28) and the quantity of emission is clear. Figure 3o shows the time pattern over the course of the day for the individual emission constituents. Tables 51 and 52 show the average emissions per litre of fuel in the area under consideration.

The absolute quantities of the emissions from traffic are given in Tables 53 - 56. These show that inorganic gases, totalling 66.ooo metric tons/year, account for the greatest proportion of vehicles emissions. Of this total, 95% is carbon monoxide, o,5% sulphur dioxide, and 4,5% oxides of nitrogen.
Hydrocarbons amount to 2.4oo metric tons/year. 2.ooo metric tons of dust emission per year are to be expected from vehicle engines; approximately half of the total is soot from trucks engines, and the other half is lead-containing constituents from cars.
The amount of tyre wear was also assessed for the area under study. For the stated total of 2.8 thousand million kilometres driven it is of the order of 5oo metric tons/year.

3. ASSESSMENT OF A SUB-AREA OF THE AREA UNDER INVESTIGATION.

3.1.

Comparison of the relative contributions of different emissions.

The assessments which have been carried out up to the present time were based on incomplete information from the entire area to be investigated (Map 1). As the extent of progress in the investigations of the three source groups-industry, road traffic, and domestic heating/small business-varies from place to place, the data relating to these sources over the area as a whole are not directly comparable. To make a comparative analysis possible, the present section of the report deals only with a particular sub-area in which the investigations of all source groups are substantially complete. Table 57 and Figure 31 show the emissions which have been determined in this sub-area, and the relative contributions of the different source groups. The following comparison of the constituents carbon monoxide, sulphur oxides, nitrogen oxides, organic gases and vapours, and dust, is based on annual emissions.

Carbon monoxide emissions in the sub-area total approximately 9o.ooo metric tons/year. Of this total, 45% is from domestic heating, 49% from traffic, and 6% from industry. Thus, carbon monoxide comes mainly from domestic heating and from traffic, in roughly equal proportions.

The total yearly emission of sulphur oxides in the sub-area under consideration is about 4o.ooo metric tons, of which 82% comes from industry and 17% from domestic heating and small business. In terms of quantity, the contribution from road traffic is negligible. Thus, sulphur oxide emissions in the sub-area are mainly from industry.

Emissions of nitrogen oxides total about 2o.ooo metric tons/year, of which the greater part (82%) is again from industry. Road traffic accounts for 1o%, and domestic heating and small business for 8%.

Emissions of organic gases and vapours in the sub-area amount to about 3o.ooo metric tons/year. 83% of these emissions are from industrial plants, 11% from domestic heating and small business, and 6 % from traffic. Emissions from the industrial source group predominate.

Dust emissions in the sub-area total about 5.3oo metric tons/year. 54% comes from heating installations in buildings and from small business, and 43% from industrial plants. Less than 3% comes from road traffic.

In the graph (Figure 31), which shows the relative contributions of the five constituent groups from the different sources, the total of the five columns is 1oo%. Over the area in question, carbon monoxide accounts for 49% of the total emission, sulphur oxides for 22%, nitrogen oxides for 11%, organic gases and vapours for 16%, and dust for 3%.

It would be possible to present this information on the relative amounts of the different emissions from the different source groups in a more revealing way by reference to unit areas 1oo metres x 1oo metres, or by the use of squared grids on which the length of one side corresponds to one kilometre on the ground. However, such a detailed presentation of the facts is unacceptable to legitimate industrial and business interests (compare § 139 b of the Factories Act). Since ist is not possible to give full details on particular emissions from particular sources, the following part of the report is restricted to a detailed consideration of the ambient air situation in the area under consideration.

3.2.

Comparison of the relative proportions of pollution constituents.

A consideration of the relative proportions of emissions from different source groups or emitters is not by itself a sufficient basis for clean air planning measures. What is of decisive importance is the resulting pollution of the air, which depends not only on the quantity of emissions but also - and to a greater extent - on the conditions of emission, particularly the height above ground level and the factors affecting diffusion.
Details of the conditions affecting emissions are given in the emissions inventory. Therefore, for a particular region under consideration, the meteorological conditions and other factors affecting the emissions must be taken into account when estimating the contribution of particular source groups or emitters to the resulting pollution load. This sort of assessment considered in relation to the permitted immission limits, makes it possible to decide on the importance of particular emission constituents, source groups, or individual emitters. This is the point of departure for rational clean air measures.

This method is illustrated for the sub-area in question by a consideration of the constituents carbon monoxide, sulphur oxides, nitrogen oxides, and organic gases and vapours when the wind is in a particular direction. For the sake of simplicity certain assumptions are made with respect to these emissions (see 3.2.1.3). The results - which in view of this simplification cannot be taken as definitive, but which do nevertheless permit conclusions at least to an order of magnitude - are set out in Maps 6 - 37. Maps 6 - 9, 14 - 17, 22 - 25, and 3o - 33 show for each constituent the pollution load at the centre point of the unit area, and the extent to which the three source groups have contributed to it. In this report no reference is made to individual emitters.

3.2.1

Basis for the calculation of pollution fields.

3.2.1.1

Diffusion model.

The use of mathematical-meteorological diffusion mode[illegible] permits calculation of the amount of pollution to be expected from specified emissions - taking into account the conditions of emission and diffusion - and determination of the contribution of individual source groups or emitters. The principles on which the diffusion models were based are to be found in (18), and a full description will not be given here. There is no doubt as to the applicability of diffusion models to the purpose under discussion (19,2o). The arithmetical model used here is intended for an area with numerous buildings, and hence with a very uneven profile.

3.2.1.2

Conditions of dispersal.

The diffusion of foreign matter in the atmosphere is determined to a large degree by the conditions of emission (initial impetus and the tendency of hot emissions to rise) and by the turbulence of the atmosphere. To calculate pollution levels it is necessary to determine, from meteorological records, diffusion classes which take into account all factors affecting turbulence. Table 58 gives the frequency distribution of diffusion class and wind speed, based on a scheme described by Klug (3) (see page 2o), using data collected by the Cologne-Bonn weather station over a period of five years. Table 59 shows the frequency distribution of wind directions over the same period of time. A complete explanation of the three-dimensional frequency distribution of diffusion class, wind direction, and wind speed will not be given in this report.

Up to the present time, the emissions list includes the emissions of the Dormagen area, the north of Cologne, and the city centre, including the west (Map 4). It can be assumed that all important emissions affecting the pollution load of the sub-area in question when the wind is between north and north-west are recorded in the list; if one excludes long distance effects of the areas around Mönchengladbach and possibly Neuss. The combination of emission sources when the wind is from this quarter is typical of a conurbation with a city centre at its middle, industrial areas at the periphery, and other residential areas between. The diffusion calculation was therefore based on the assumption of a north-northwesterly wind (335°), which, admittedly, occurs in only about 2.5% of the hours in a year (see page 19). This situation is a striking example of the diffusion of air pollutants in a conurbation, but does not permit any conclusions relating to the total pollution load in such an area. For this, one needs an assessment of a larger area, with all wind directions taken into account. An assessment of this sort will be carried out in the Cologne area when the emissions inventory programme is complete (see page 15).

Emmissions from domestic heating and small business, and also from road traffic, depend on the season and the time of day. Therefore, in calculation immission levels, a distinction is made between winter and summer, and day and night. For the sake of the example under consideration, particular diffusion situations were selected. According to (21) it can be assumed that during the night there are for the most part (60%) stable conditions of diffusion (Classes I and II, low turbulence), and relatively low wind speeds. During the day the diffusion conditions are mostly (75%)"neutral" (Classes III_1 und III_2, middle turbulence), generally with higher wind speeds. In the light of these facts, Class II with a wind speed of 2 metres/second was chosen to represent the night situation, and Class III_1 with a wind speed of 4 metres/second to represent the day situation.

3.2.1.3

Conditions of emission.

In the calculations, the individual emission sources industry, road traffic, and domestic heating/small business were taken to be spatial, line, or point sources.

Emissions from domestic heating and small business were calculated on the basis of area sources 1.ooo metres square. The average chimney height was taken to be 15 metres, with an effective height of emission assumed to be 2o m.

Emissions from traffic -without the exception of thonse from autobahns and fast roads without buildings- were regarded as area sources 1ooo metres x 1ooo metres. Autobahns and fast roads without buildings, were taken as line sources with an emission height of Ometres. For the emission height of area sources the average height of the buildings - approximately 15 metres - was taken. By this approach it is the resulting contributions to pollution over the area which are measured, and not the immissions in the streets themselves. This is the correct approach for an overall determination of the area-related immission. The concentrations determined in this way are valid for all parts of the area, with the exception of the 'street canyons' themselves up to the height of the adjacent buildings.
The pollution levels of the relevant constituents in the street canyons themselves may be greater to the extent of orders of magnitude, as will become apparent in the discussion of results.

Among the industrial sources, two groups are distinguished. Those below a height of 5o metres were regarded as area sources 1.ooo metres x 1.ooo metres, emitting at a height of 25 metres. To take into account the rise of columns of waste gas, an effective height of emission of 35 metres was assumed. High level industrial sources, which were without exception chimneys emitting at a height above 5o metres, were noted from the emissions inventory as individual sources. The extent to which the colums of waste gas rose above this level was calculated by the method of Briggs (22).

Overall treatment of particular groups of sources, by evening out the grouping of sources, introduce errors into the diffusion calculation, but these do not significantly affect the accuracy of the results.

In view of the differing extents to which emissions depend on the season and the time of day, four different situations were selected. The breakdown by season and time of day is as follows:

Summer, during the day --------------Situation A
Summer, at night --------------------Situation B
Winter, during the day --------------Situation C
Winter, at night --------------------Situation D

The time dependence of the emissions, taken into account in the calculations, is shown in table 6o, which expresses hourly emissions at a particular time as a proportion of the average hourly emission over the whole year. The yearly figures were calculated from the annual emission figures for the 1.ooo metres x 1.ooo metres grid areas in Map 5. The following two examples will serve to explain the table. During the day the hourly emission from traffic is greater by a factor of 1.5 than the hourly average over the year. Emissions from domestic heating and small business - with the exception of organic gases and vapours - are negligible in summer, especially during the night.

3.2.2

Results of the pollution calculations.

The immission figures were calculated as hourly averages for the points of intersection of the 1.ooo metres-square grid areas on Map 5. The results are presented in different ways, as follows:

1. The concentration of pollution (µg/m^3) at the centre point of the unit area, with an indication of the relative contributions of the three source groups (Maps 6 - 9, 14 - 17, 22 - 25, and 3o - 33). Concentrations below 1 µg/m^3 are not stated numerically.

2. 'Contours' of equal concentration (µg/m^3) of immission for the sub-area (Maps 1o - 13, 18 - 21, 26 - 29, and 34 - 37).

3. A section across the field of concentration, in the direction of the wind, starting from Dormagen (vertical grid 5.662.5/ horizontal grid 2.558.o) (Figures 32 - 35).

As was stated in 3.2.1.3, this presentation of the results is not concerned with the pollution in the street canyons (discussed in 3.2.3).

3.2.2.1

Carbon monoxide.

In the presentation (Maps 6 - 9) of the percentage contributions of the source groups giving rise to carbon monoxide pollution it is clear that - particularly in situations A and B (summer) - the level of pollution is determined almost exclusively by emissions from traffic. This is because in summer the contribution from domestic heating is negligible. On the other hand, the carbon monoxide maps for situations C and D (winter) show substantial contributions from domestic heating.

The 'contours' of equal concentration (Maps lo - 13) show the important role of traffic in the vicinity of fast roads and autobahns, particularly in the area of the Cologne-North autobahn crossing. In all the situations which were calculated, the maximum concentrations were found in the city centre of Cologne. In situation D (during the night), in winter), pollution concentrations above $1mg/m^3$ are to be expected in the Southern part of the city centre.

Figure 32 shows the build-up of carbon monoxide concentration within the Cologne city area. In both summer situations (A and B), concentrations in the region of o.4 mg/m^3 are reached. Curves A and B show that the immission levels at night and during the day are practically identical. In spite of the fact that, during the night, emissions are less by a factor of 3—4, the more stable weather situation permits the pollution to accumulate to the same level as during the day. The contribution of domestic heating emissions during the winter raises the carbon monoxide concentration during the day by about o.5 mg/m^3, and during the night by as much as o.9 mg/m^3.

3.2.2.2

Sulphur oxides.

Maps 14 and 15, giving the percentage contributions of the source groups to sulphur oxide pollution in summer, show the heavy contribution from industry, and the nil or minimal contribution from domestic heating and traffic. In winter, as Maps 16 and 17 show, the pollution comes mainly from domestic heating emissions, particularly in the city centre of Cologne. At night time the concentrations are nearly three times as high as during the day, despite the smaller quantities emitted, supposedly because conditions during the night do not favour diffusion. In Cologne, the average concentration of sulphur oxide pollution during the night is about 2o% lower than during the day (23).

The 'contours' of equal concentration over the sub-area in question (Maps 18 - 21) show the effect of individual industrial sources in the north. On the basis of the diffusion situation which is assumed to prevail during the night, relatively high concentration persist up to considerable distances.

The distribution of sulphur oxide concentrations along the longitudinal sections form Dormagen to Cologne City Centre (Figure 33) is different from that for carbon monoxide (Figure 32), because the emission situation for sulphur oxides is entirely different. In Worringen, for example, the effect of the industrial region to the north is noticeable. Unlike situation A (summer, during the day), when the conditions for diffusion are favourable, curve B shows the situation during a summer night, when, because of the unfavourable diffusion situation, higher concentrations are built up and sustained along the direction of the wind, despite the fact that the quantity emitted is approximately the same. The effect of domestic heating in winter is shown in curves C and D. When conditions do not favour diffusion, the concentration in the city area rises to o.25 mg/m^3 during the day (situation C), and o.35 mg/m^3 during the night (situation D). Because emissions from vehicles are minimal, traffic does not perceptibly affect the level of sulphur oxide pollution.

3.2.2.3

Nitrogen oxides.

Maps 22 - 25, giving the percentage contributions of the three sourcegroups to nitrogen oxide pollution, show clearly the predominant effect of the industrial sources to the north. In the city centre of Cologne, traffic is an important source. In winter the contribution of the domestic heating/ small business source group is relatively greater.

Maps 26 - 29, giving the 'contours' of nitrous gas pollution, show the effect of the industrial sources to the north, and, within the area of Cologne city, the influence of domestic heating and small-scale industry.

As can be seen from curve C in Figure 34, there is during the daytime in winter - along the Dormagen/Cologne axis, within the city area - additional pollution to an extent of about 2o µg/m^3 from domestic heating.
During the night, when conditions are less favourable for diffusion, the concentration of nitrous gases in the city of Cologne is 3 - 4 times greater than in the day. Here again, the influence of industry in the north is clear, and this declines only gradually during the night. The drop in concentration along the Dormagen/Cologne axis is overlain by the contribution from traffic, although the level of emission from this source is relatively low.

3.2.2.4

Organic gases and vapours.

Maps 3o - 33, giving the percentage contributions of the source groups to organic gas and vapour pollution, show heavy contributions from industry, particularly during the night when the conditions do not favour diffusion (situations B and D). In the winter, when heating is on, domestic heating also has a detectable effect within the city of Cologne, particularly during the day. The relatively heavy contribution of the domestic heating/small business sub-group during the summer (situation A) is attributable to the emissions of small-business (e.g. petrol stations, dry cleaning establishments).

Maps 34 - 37 show 'contours' of equal pollution load, and clearly indicate the dominant influence of the industrial sources to the north. Figures 35 points to the same conclusion.

3.2.3

Pollution in street canyons.

In the diffusion model, traffic is assumed to emit at a height of 15 metres above the ground, so that the calculation gives the level of pollution to be expected outside the street canyons.
To be able to compare the pollution contributions of the three source groups, it is therefore necessary to estimate the amount of pollution from traffic at street level, or determine it by measurement.

Measurements were taken in a number of streets in the city centre of Cologne. Guthoff and Deimel (23) have published measurements taken at a level of 1.5 metres above ground, generally at points 1o - 15 metres before traffic lamps. These relate to traffic in streets flanked by buildings of various heights, during the period between 6.oo and 2o.oo hours. Individual measurements were taken for periods of 9o minutes on each occasion, on a total of at least nine different days during the summer/winter period.
The average number of vehicles per 3o minutes was recorded, in addition to the average and maximum half-hourly carbon monoxide concentrations. The published values are to be understood as having been statistically selected: there is no systematic analysis or arrangement of the wind conditions in the street or above the level of the buildings. The Rhineland Technical Supervisory Committee carried out measurements over 14-hour periods on at least two days in 13 different roads. The measurement sites were wherever possible situated between two crossings, in order to reduce the effect of the traffic building up before the crossings. Measurements were taken at

o.75, 1.5, 3.o, and 4.5 metres. The readings at the different heights depend on the amount of building alongside the road, and the amount of ventilation in the road up to the height of the adjacent buildings. If the ventilation remains steady, the concentrations at o.75 metres and 1.5 metres generally do not differ by more than 2o - 25%. The effects of wind direction and wind speed sometimes produce a scattering of the results. However, these effects will not be taken into account in the present comparison.

In Table 61 the results of measurements are compared with the calculated level of pollution from the three source groups industry, domestic heating/small business, and traffic, in the day/night summer/winter situations defined in 3.2.1.

The differences in the average and maximum concentrations in the two series of measurements (Table 61) are explicable in terms of the different situation of the measurement sites, and the wind conditions - or rather the extent to which these bring about diffusion of the emissions in the street canyons. Leaving out of account the fact that these measured concentrations differ by a factor of 2, it is apparent from the table that the level of pollution from the three source groups outside the confines of the street represents $\frac{1}{5}$ down to $\frac{1}{1oo}$ of the local pollution load from the traffic.
This difference is reduced by a factor of lo or less under the diffusion conditions which are assumed to exist during the night. The stated night-time concentrations after 22.oo hours were obtained by extrapolation.

To compare the impacts of pollutions such as sulphur oxides, nitrogen oxides, and organic gases and vapours, produced in the street by the traffic, the quantities of these pollutants were calculated from the measured quantities of carbon monoxide by the use of the conversion factors below. Naturally, considerable uncertainty attaches to this method, but it should be accurate enough to assess - to an order of magnitude - the pollution occurring at street level as a result of emissions from traffic, as opposed to the pollution from distant sources which is diffused over a wider space.

The results for sulphur oxides, nitrogen oxides, and organic gases and vapours are given in Tables 62 - 64.

In the street canyons, the sulphur oxide pollution (Table 62) from traffic - estimated by use of the conversion factors given above - in diffusion situation A (summer) is comparable with that from outside sources. In all other situations the pollution from other sources is 5 - lo times as great.
The stated average readings of sulphur oxide concentration are comparable with the calculated immission for the individual situation.

The estimated level of traffic-generated nitrogen oxide pollution (Table 63) in the street during the day is about lo - 3o times greater than the calculated concentration outside the street. The concentrations during the night are comparable with those resulting from night diffusion situations B and D.

Hydrocarbon immission at street level during the day, resulting from the traffic in a particular street, is 5 - lo times greater than that which is calculated to result from outside pollution from the three source groups under diffusion situations C and D.
The night-time pollution levels calculated on the basis of the defined diffusion situations are comparable with the estimated night-time concentrations.

Chapter XI

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The Role of Diffusion Models in a Strategic Concept for Air Pollution Control

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The role of diffusion models in a strategic concept for air pollution control

This paper was prepared for a workshop session on "Applications of Modeling and Users' Needs." It includes discussion of various practical questions of modeling ranging from the model inputs to the various uses that are made of the output.

1. Role of the model in a strategic concept for air pollution control.

May I first give you an idea of where, in my opinion, the model is located in a strategic concept for air pollution control in air quality regions. In the graph (Fig. 1) you can see the various kinds of proposed use of the model. I say "proposed" because we are in the process of implementing the scheme. The scheme shows three main applications of the model:

First: calculation of an air quality inventory (immission inventory); the inputs are the emission inventory and the meteorological conditions.

Second: calculation of the concentrations of air pollutants due to the emissions of a new industrial plant in the license procedure (immissions forecast).

Third: calculation of buffer-zone distances for the purpose of protection against air pollution in town and regional planning.

As a fourth application I suggest the analysis of polluters in the case of emergency local pollution events e.g. breakdown of gas cleaning equipment.

The central input for all the cases of model use is the emission inventory. Therefore I would like to brief you on the system, method and goals of the emission inventory which was developed by us and the Rhineland Technical Supervisory Association in Cologne. At the last NATO/CCMS meeting(1) I promised you a written report on the emission inventory Cologne; the report(2) is now presented to you with an english translation of the text.

2. Definition of an emissions inventory.

An area emissions inventory is a record of all sources of air pollution in that area, classified according to geographical position (Gauss-Krüger Coordinates) and the conditions affecting their emission (dimensions of the source; quantity and temperature of waste gases; nature and quantity of pollutant material; frequency and duration of emission).

There are point sources (for example, factory chimneys), line sources (for example, columns of vehicles on roads), and area sources (of which a good example might be the chimneys of a residential area).

An electronic data-processing system is required for the proper storage of the data. Details of how to draw up an emissions inventory and how to use it have already been published (3; 4; 5).

2.1 Drawing up an emissions inventory.

When starting to compile an inventory, the sources to be considered are industry, domestic heating, minor industry, and traffic. Various methods are used. In industry, the variety of different sources and the large number of pollutant chemicals make it necessary to employ experts to investigate each individual plant. For domestic heating and traffic an overall approach generally suffices.

2.11 Industry.

In industry, the enquiry begins at the plant from which the emission originates. All emissions from the plant are taken into account, including those from clearly defined sources and those from diffuse sources, and without regard to whether they are of such a nature - or are present in such quantity - as to contribute to pollution of the atmosphere. Whether a particular constituent is of significance as an atmospheric pollutant in a particular area becomes clear later when the inventory is assessed. The essential data relate to sources, plants and emissions.

The enquiry is carried out by technical experts who collaborate with plant management and enter their findings on the cards. The methods used for the determination of the quantities of material and the concentration of emissions range from rough assessment to selective measurement. In industry the inventory should be kept up to date mainly with data supplied by plant management under the licensing procedures of the Factories act, or obtained by technical experts when they return for later inspections. The draft of the Federal Immissions Protection Act provides that the Manager of a plant which requires approval shall provide an annual declaration of emissions, which is to be entered in the Emissions Inventory.

2.12 Domestic heating and small-scale industry.

There is no doubt that the majority of emissions from domestic heating and small-scale industry result from combustion. The nature of the emissions and the amount per unit area can be determined by an overall approach. However, emissions from small business which do not result from combustion must be determined individually, as is the case in industry.

Nevertheless, the procedure can be greatly simplified on the basis of experience. To determine the emissions from combustion in domestic fires and small business, the first step is to ascertain the quantities of the various fuels used. When this has been done, specific emission factors are used to determine the emitted quantities (per unit area) of the relevant constituents. The fuel consumption per unit area, and the heights of the chimneys, are obtained from the records which the district chief sweep is legally obliged to keep. Officially recorded data are not sufficient to ascertain the total quantity of fuel per unit area, subdivided into coal, lignite, oil, and gas. Difficulties commonly arise, particularly in the case of apartments heated by a single stove, and these can only be overcome by sample enquiries. Here again the district chief sweep can give valuable help.

2.13 Traffic.

Investigations of emissions from traffic can generally be restricted to road traffic. Emissions per unit area are most easily determined as a function of the quantity of fuel consumed. Fuel consumption per unit time depends on the number of vehicles, their engine capacity or load category, and the operating pattern. Records of numbers of vehicles are obtained by counting at particular points, or from aerial photographs taken at various times. Operating patterns are studied by the use of test vehicles, fitted with recording equipment, which are driven through the area under study in all typical traffic situations. If the operating patterns are classified in categories, and if these are simulated on engine test benches or on roller test beds with representative vehicles, it is possible to determine the emission factors of the various exhaust gas constituents as a function of the pattern of operation. The emissions per hour per unit area can be determined from the number of vehicles per hour, using the emission factors.

3. Evaluation of the emissions inventory.

An area inventory of the kind described provides the necessary basis for detailed local statements and for more general statements on clean air policy at the supra - regional level.

3.1 Contribution of various emission sources.

For given zones within the area under investigation the emissions inventory provides an overall view of the contribution of individual emission sources or groups of sources to the total emission of particular constituents. The diffusion calculation makes it possible to work out the degree of pollution by a given constituent at particular points in the area.

3.2 Basis for improvement plans.

Consideration of the relative proportions of individual constituents of immission lead to local and supra-regional conclusions regarding necessary improvements and precautionary programs. Diffusion calculations show the sources or groups of sources on which an improvement order will have the most lasting effect. If the costs of improvements and the advantages to man and the environment are taken into account, the emissions inventory can serve as the starting point for cost-benefit analyses. If the inventory showed that a particular type of pollution source is of predominant importance in densely populated areas, changes in the law could follow.

3.3 Analysis of polluters.

When there is a sudden, unexpected build-up of pollution, giving rise to public anxiety or to damage, meteorological data and dispersal calculations can be used to determine which of the listed sources is responsible.

3.4 Tool for license procedures.

In the license procedure for industrial plants the inventory of existing sources is considered in conjunction with the inventory of proposed new sources submitted for approval, and the dispersion calculation then shows the pollution which would result from the new plants at any chosen point in the affected area. It is also possible to calculate what improvements are needed in existing plants to ensure that the construction of new plants does not bring the total pollution above the accepted limit.

3.5 Assistance for town and regional planning.

In city and regional planning the emissions list, together with dispersal calculations, serves to determine the necessary distance between existing residential areas and new industrial areas, or vice-versa, depending on the emissions from the industry. When assigning an area for industrial use, the existing or simulated inventories would have to be transplanted for siting.

3.6 Planning of air quality measurements.

The emissions inventory provides pointers as to which constituents of an emission are relevant from the standpoint of pollution. Dispersal calculations are easier and more reliable when particular points are established for the taking of measurements. The chosen points are those at which the highest concentrations of the particular emission constituent are expected, and this technique avoids the expensive measurement on an area basis by "the rule of thumb."

4. Application of a diffusion model in Cologne.

The emission inventory of the Cologne area is not yet complete. Nevertheless we used some of the described ways of evaluating the inventory, and specifically we tried to convert the emission inventory into an air quality inventory (immission inventory).

A consideration of the relative proportions of emissions from different source groups or emitters is not by itself a sufficient basis for clean air planning measures. What is of decisive importance is the resulting pollution of the air, which depends not only on the quantity of emissions but also - and to a greater extent - on the conditions of emission, particularly the height above ground level and the factors affecting diffusion.

Details of the conditions affecting emissions are given in the emissions inventory. Therefore, for a particular region under consideration, the meteorological conditions and other factors affecting the emissions must be taken into account when estimating the contribution of particular source groups or emitters to the resulting pollution load. This sort of assessment considered in relation to the permitted immission limits (air quality standards), makes it possible to decide on the importance of particular emission constituents, source groups, or individual emitters. This is the point of departure for rational clean air measures.

This method is illustrated for the sub-area in question by a consideration of the constituents carbon monoxide, sulphur oxides, nitrogen oxides, and organic gases and vapours when the wind is in a particular direction. For the sake of simplicity certain assumptions are made with respect to these emissions.

4.1 Simplified conditions of emission.

In the calculations, the individual emission sources, industry, road traffic, and domestic heating and small business were taken to be spatial, line, or point sources.

Emissions from domestic heating and small business were calculated on the basis of area sources 1.ooo metres square. The average chimney height was taken to be 15 metres, with an effective height of emission assumed to be 2o m.

Emissions from traffic - with the exception of those from autobahns and fast roads without buildings - were regarded as area sources 1ooo metres x 1ooo metres. Autobahns and fast roads without buildings, were taken as line sources with a zero emission height. For the emission height of area sources the average height of the buildings - approximately 15 metres - was taken. By this approach it is the resulting contributions to pollution over the area which are measured, and not the immissions in the streets themselves. This is the correct approach for an overall determination of the area-related immission. The concentrations determined in this way are valid for all parts of the area, with the exception of the 'street canyons' themselves up to the height of the adjacent buildings. The pollution levels of the relevant constituents in the street canyons themselves may be greater to the extent of orders of magnitude.

Among the industrial sources, two groups are distinguished. Those below a height of 5o metres were regarded as area sources 1.ooo metres x 1.ooo metres, emitting at a height of 25 metres. To take into account the rise of columns of waste gas, an effective height of emission of 35 metres was assumed. High level industrial sources, which were without exception chimneys emitting at a height above 5o metres, were noted from the emissions inventory as individual sources. The extent to which the columns of waste gas rose above this level was calculated by the method of Briggs.

Overall treatment of particular groups of sources, by evening out the grouping of sources, introduce errors into the diffusion calculation, but these do not significantly affect the accuracy of the results.

In view of the differing extents to which emissions depend on the season and the time of day, four different situations were selected. The breakdown by season and time of day is as follows:

Summer, during the day
Summer, at night
Winter, during the day
Winter, at night

The time dependence of the emissions, taken into account in the calculations, is expressed by hourly emissions at a particular time as a proportion of the average hourly emission over the whole year. The yearly figures were calculated from the annual emission figures for a 1.000 metres x 1.000 metres grid.

4.2 Diffusion model.

The mathematical model used here is intended for an area with numerous buildings, and hence with a very uneven profile. The model will be described in the sessions tomorrow by Dr. Bresser.

4.3 Conditions of dispersal.

Up to the present time, the emissions list includes the emissions of the Dormagen area, the north of Cologne, and the city centre, including the west. It can be assumed that all important emissions affecting the pollution load of the sub-area in question when the wind is between north and north-west are recorded in the list, if one excludes long distance effects of the areas around Mönchengladbach and possibly Neuss. The combination of emission sources when the wind is from this quarter is typical of a conurbation with a city centre at its middle, industrial areas at the periphrey, and other residential areas between. The diffusion calculation was therefore based on the assumption of a north-northwesterly wind (335°), which, admittedly, occurs in only about 2.5% of the hours in a year. This situation is a striking example of the diffusion of air pollutants in a conurbation, but does not permit any conclusions relating to the total pollution load in such an area. For this, one needs an assessment of a larger area, with all wind directions taken into account. An assessment of this sort will be carried out in the Cologne area when the emissions inventory programme is complete.

Emissions from domestic heating and small business, and also from road traffic depend on the season and the time of day. Therefore, in calculation of emmission levels, a distinction is made between winter and summer, and day and night. For the sake of the example under consideration, particular diffusion situations were selected. It can be assumed that during the night there are for the most part (60%) stable conditions of diffusion (Classes I and II, low turbulence), and relatively low wind speeds. During the day the diffusion conditions are mostly (75%) "neutral" (Classes III_1 und III_2, middle turbulence, generally with higher wind speeds. In the light of these facts, Class II with a wind speed of 2 metres/ second was chosen to represent the night situation, and Class III_1 with a wind speed of 4 metres/second to represent the day situation.

4.3 Results of the pollution calculations.

The immission figures were calculated for CO, SO_x, NO_x and HC as hourly averages for the points of intersection of the 1.ooo metres-square grid areas. The results are presented in different ways, as follows:

1. The concentration of pollution ($\mu g/m^3$) at the centre point of the unit area, with an indication of the relative contributions of the three source groups (Maps 6 - 9, 14 - 17, 22 - 25, and 30 - 33 in the reference (2)). Concentrations below 1 $\mu g/m^3$ are not stated numerically.
2. 'Contours' of equal concentration ($\mu g/m^3$) of immission for the sub-area (Maps 1o - 13, 18 - 21, 26 - 29, and 34 - 37 in the reference (2)).
3. A section across the field of concentration, in the direction of the wind, starting from Dormagen (vertical grid 5.662.5/ horizontal grid 2.558.o) (Figures 32 - 35 in the reference (2)).

Maps and figures are not reproduced here. Please refer to reference (2)). As was stated this presentation of the results is not concerned with the pollution in the street canyons.

5. Defining buffer zone distances by use of diffusion model.

One of the most inportant decisions in taking account of the factor of air pollution control in town and regional planning and in the licensing procedure for industrial plants is the fixation of distances between residential areas on the one hand and industrial areas on the other. Those decisions can be based on calculations in the special case or on so-called buffer zone lists. I made a proposal for defining such distances in special cases (3) and - in cooperation with Dr. Bresser- for the standardization in buffer zone list (6).

The proposal is based on the possibility to calculate, for given emission situations (emission inventory), the corresponding air pollution concentrations (immissions) in the vicinity of an emitting plant by means of mathematical-meteorological diffusion model. We use the model described by Dr. Bresser in section II of the session.

The emission inventory for existing plants will be established like the description in part 2 of my presentation and in reference (4). Emission inventory for proposed plants can also be established by representing the exact operational planning according to the methods of establishing emission inventory.

There are two problems involved in defining the required protective distance between emitting industry and residential areas:

a) the evaluation of the facts, i.e. to find out according to type, concentration and frequency what air pollution concentrations (immissions) occur in the surrounding residential areas, and

b) the assessment of the facts, i.e., to decide what immissions by type, concentration and frequency can be tolerated in the residential areas.

The first problem can be solved by calculation of diffusion in connection with emission inventories. Air quality standards (maximum immission concentrations) are required for assessing the facts evaluated in this way.

The only difference in defining protective distances in the individual case and for establishing buffer zone lists lies in the fact that the emission inventory and the meteorological conditions must be "standardized" for specific industrial plants on the one hand and for specific regions on the other. We need

> "standard emission inventories" and
> "standard meteorologic conditions."

In reference (3) is given an example for the individual case, in reference (6) an example for the standardization of protective distances.

6. Conclusions.

Diffusion models are an important instrument in modern strategic concepts for air pollution control. The importance of diffusion models is rapidly growing in Germany.

References

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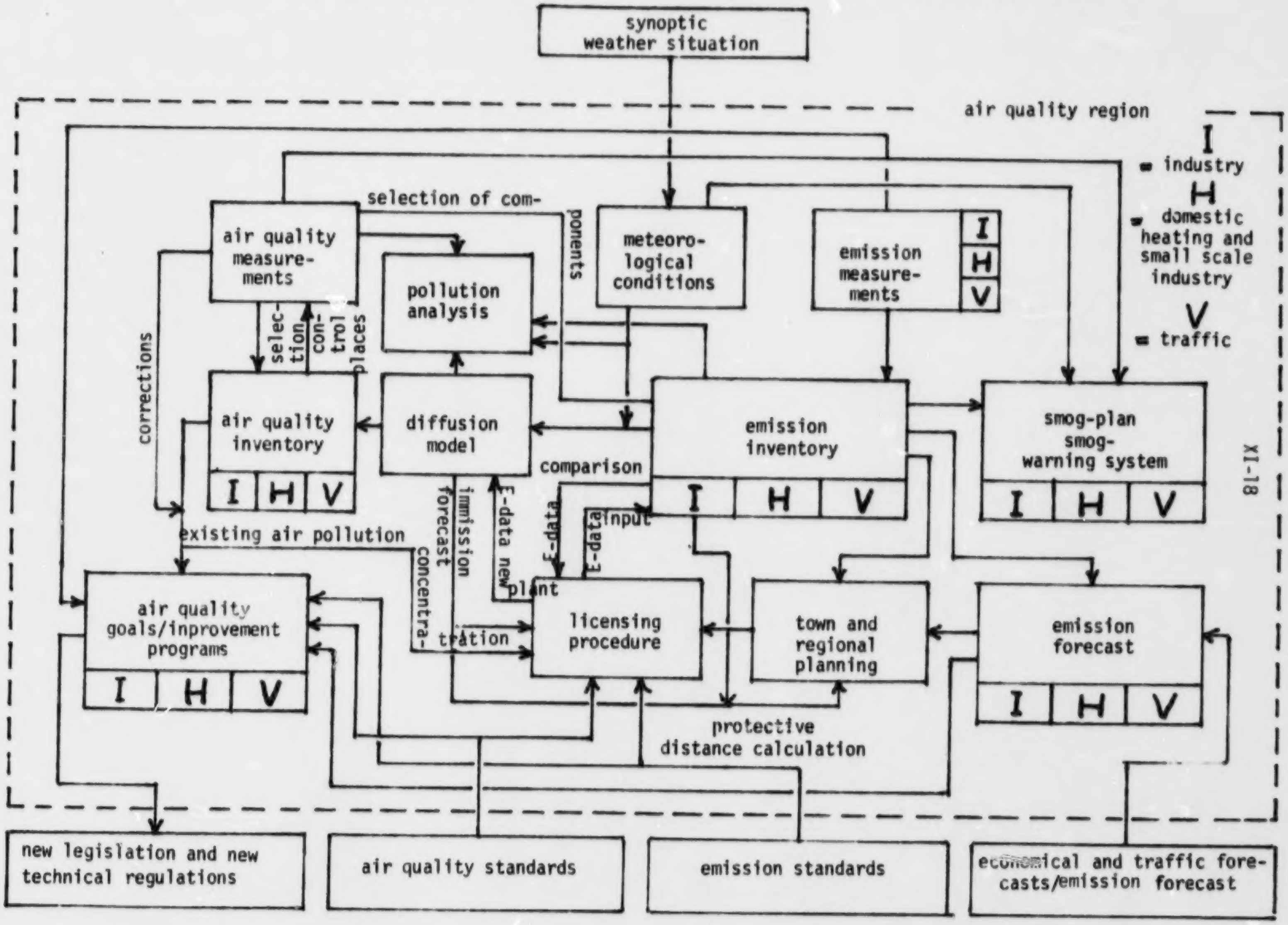
(6) F. J. Dreyhaupt und E. Plassmann: Schutzabstände als Instrument der Stadt- und Regionalplanung zur Berüsksichtigung des Faktors Luftreinhaltung - ein Beitrag zur Abstandsnormierung-, Verlag TÜV Rheinland, Köln, 1972.

Fig. 1: Scheme of a strategic concept for air pollution control in air quality regions


synoptic weather situation
air quality region
I = industry
H = domestic heating and small scale industry
V = traffic
air quality measurements
selection of components
pollution analysis
meteorological conditions
emission measurements
I H V
selection
control places
corrections
air quality inventory
I H V
diffusion model
emission inventory
I H V
smog-plan smog-warning system
I H V
comparison
existing air pollution
immission forecast
concentration
E-data new plant
E-data
E-data input
air quality goals/inprovement programs
I H V
licensing procedure
town and regional planning
emission forecast
I H V
protective distance calculation
new legislation and new technical regulations
air quality standards
emission standards
economical and traffic forecasts/emission forecast

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Dispersion Model Used in the Cologne Region

NATO/CCMS
May, 28. - 30. 1973
Oberursel

Dispersion Model used in the Cologne Region

The increasing of population on the one hand and of industry on the other and the lack of sufficient free space in our country to settle new industries make town and regional planning necessary. By planning the use of certain areas at the right time a nearly nonreversable damage can be avoided. A means to do reasonable planning is the estimation of air quality influenced by industrial plants, for instance, by the use of a practicable dispersion model. Calculations of the air quality can be done if an emission register of industrial plants or even a region is available.

The mathematical basis of the model used by us is the well known equation with gaussian distributions of the concentration normal to the axis of transport.

Turbulence due to meteorology and topography is described by corresponding parameters.

For the application of this model several assumptions are necessary:

1. The pollution must be gaseous or behave like gases. So, dust should have a grain size smaller than 10 μm. Transport is done by the air with the wind in a homogenous wind field.

2. Emissions must be constant with time and pollution does not suffer any physical or chemical change.

3. Plume pollution does not suffer any absorption at the ground, i.e. total reflection is assumed.

4. The different sources do not have an influence on each other and may therefore be superposed.

The calculation of plume rise is done using Brigg's formula. The wind speed responsible in the range of dispersion is set equal to the mean wind speed between the stack height and the effective source height. The dependance of the wind speed with height is described by the known potential law. The exponent depends on the different turbulence classes. The dispersion of emissions from line or area sources is described by modified diffusion parameters as follows:

$$\sigma = \sqrt{\sigma_0^2 + \sigma_1^2}$$

where σ_0 is the diffusion parameter due to atmospheric turbulence and σ_1 simulates an initial state of dispersion of line or area sources, so $4.3\ \sigma_1$ equals to the width of the projection of an area source onto the normal to the drift direction. One practical application of the model was used for the estimation of buffer zone distances as for instance around a standard refinery with a capacity of about 10 million tons of crude oil. Using the threedimensional statistical distribution of wind speed (10 ranges of wind speed), wind direction (36 sectors of 10 degrees) and turbulence class (6 classes of turbulence) measured in the Cologne region the frequence of excess of defined air quality standards was calculated around the plant. Diffusion parameters used for this calculation where those to be valid for a region with roughness due to buildings, plants or forests.
Fig. 1 shows the results of this calculation. With a limit of injury of 2.9 mg/m^3 for organic gases and vapours a buffer zone distance around this plant of 1700 meters was derived for an excess frequency of 1 %.

Another application of model calculations was done during the study on emissions in the Cologne region. This study was already mentioned by Dr. Dreyhaupt. Emissions from industry, from domestic heating as well as from road traffic were taken together to form area sources of 1 km side width for each source group since emission height was less than 50 meters. Emissions from road traffic along the highways were handled as line sources. Road traffic's emission height within the city was set to 15 m and emission height of domestic heating was set to 20 m where plume rise is included.

Assuming one fixed wind direction (NNW) calculations of air quality, in our case of carbon monoxid (CO), sulfur dioxide (SO_2), nitrogene oxid (NO_x) and organic gases, were done for two turbulence situations,

i) neutral with a wind speed of 4 m/s and
ii) stable with a wind speed of 2 m/s.

These calculations were done for emission situations at the day or in the neight. Only a few examples can be presented here.

Fig. 2 *) shows the expected air quality for neutral turbulence conditions due to SO_2-emissions at a day in summer.

Fig. 3 *) shows the same for SO_2-emissions conditions in the winter.

The amount of industrial and domestic heating influence, respectively. is shown by different colours. The influence of road traffic is very low, so it cannot be seen here.

Fig. 4 *) shows the same SO_2-calculation as fig. 3 *) demonstrating the air quality to be expected by lines of constant concentrations.

*) The figures 2, 3 and 4 correspond to"Karte 14", "Karte 15" and "Karte 20" of the publication "Emissionskataster Köln" given by Dr. Dreyhaupt.

Another kind of display is to be seen in fig. 5. It is the concentration of carbon monoxide (CO) along a line parallel to the drift direction drawn for four different situations of turbulence and emission:

Slope A - emissions at a summer day
neutral turbulence and 4 m/s wind speed

Slope B - emissions at a summer neight
stable turbulence and 2 m/s wind speed

Slope C - emissions at a winter day
neutral turbulence and 4 m/s wind speed

Slope D - emissions at a winter neight
neutral turbulence and 2 m/s wind speed.

The dependance of air quality with distance shows the strong influence of road traffic at about 13 km. The influence of domestic heating in the winter is to be seen in the slopes C and D. Curve D is heigher than curve C because of the more stable turbulence of the atmosphere and the lower wind speed, though the emission of domestic heating is smaller in the neight than during daytime.

Further displays are given in the publication "Emissionskataster Köln" Dr. Dreyhaupt gave to you. We only were able, here, to give you a rough survey of the capabilities of the model used by us, in order to have more time for discussions.

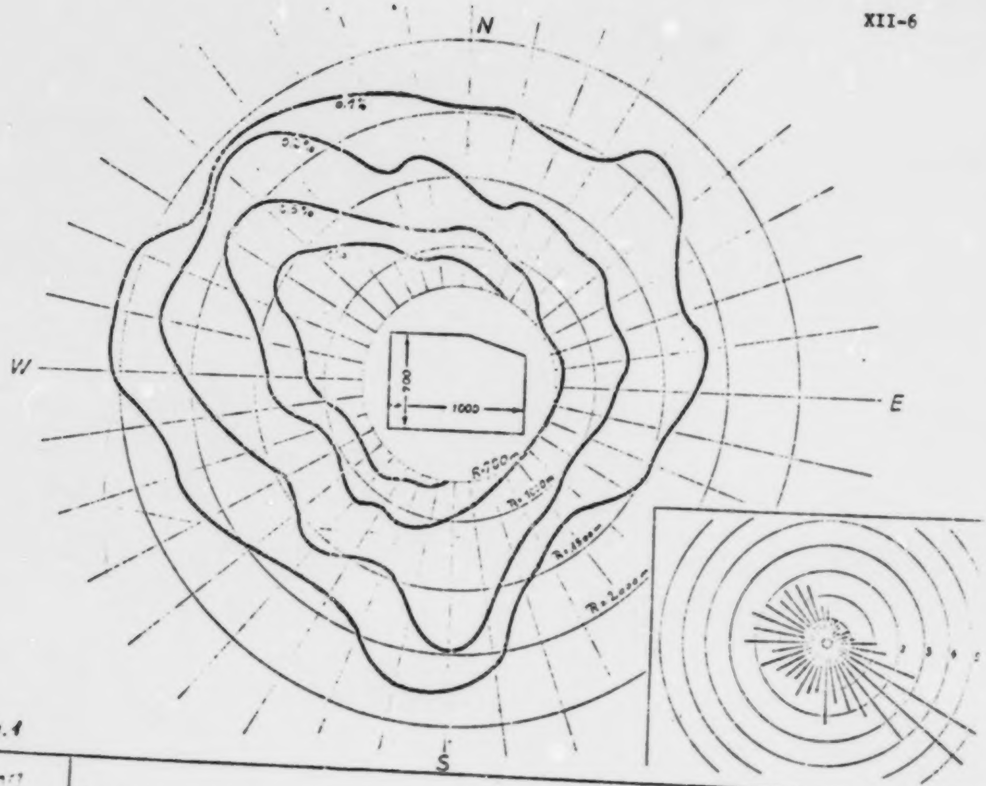

N
W
E
S
0.1%
0.2%
0.5%
1%
700
1000
R=700m
R=1000m
R=1500m
R=2000m
2
3
4
5

Fig. 1

Excess frequency of an air quality standard of 2,9mg/m³ around a chemical plant	7321

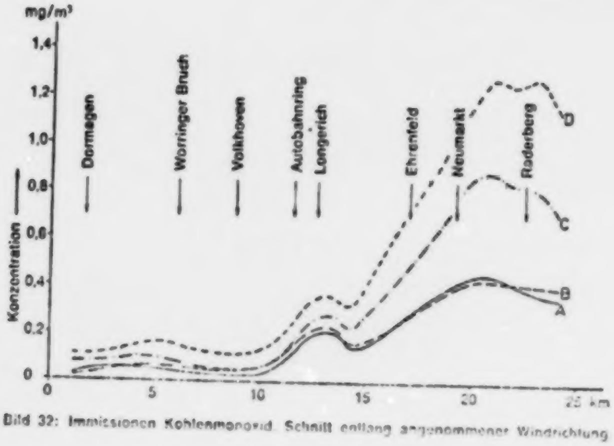
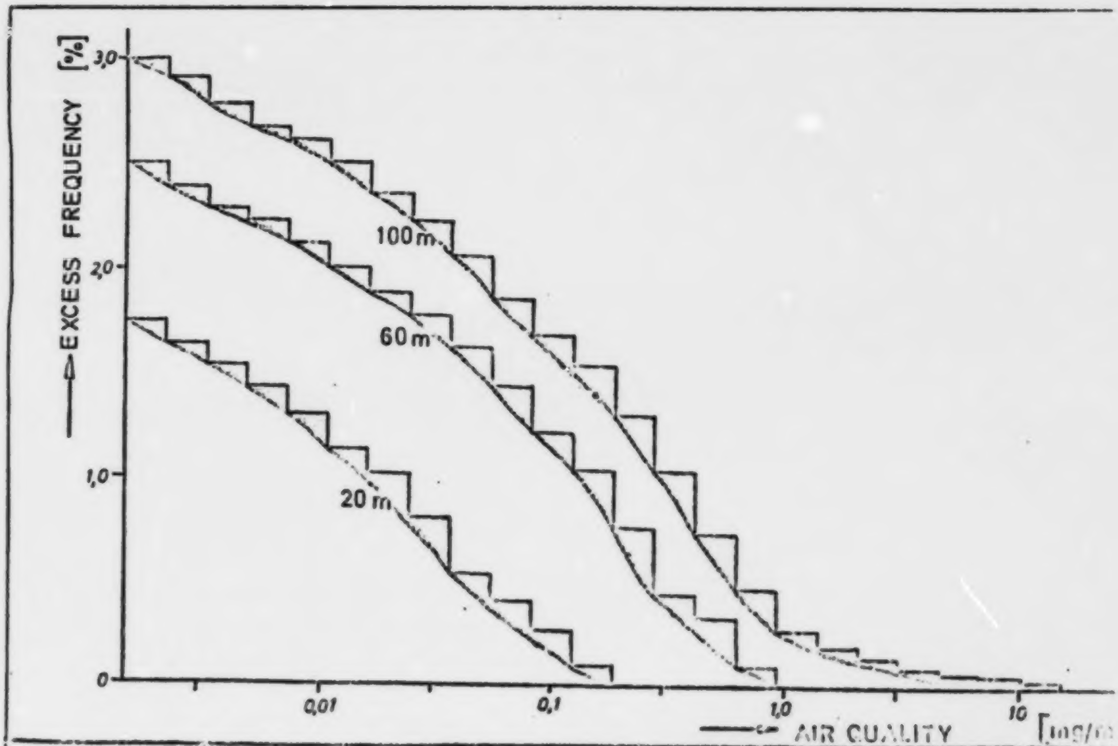


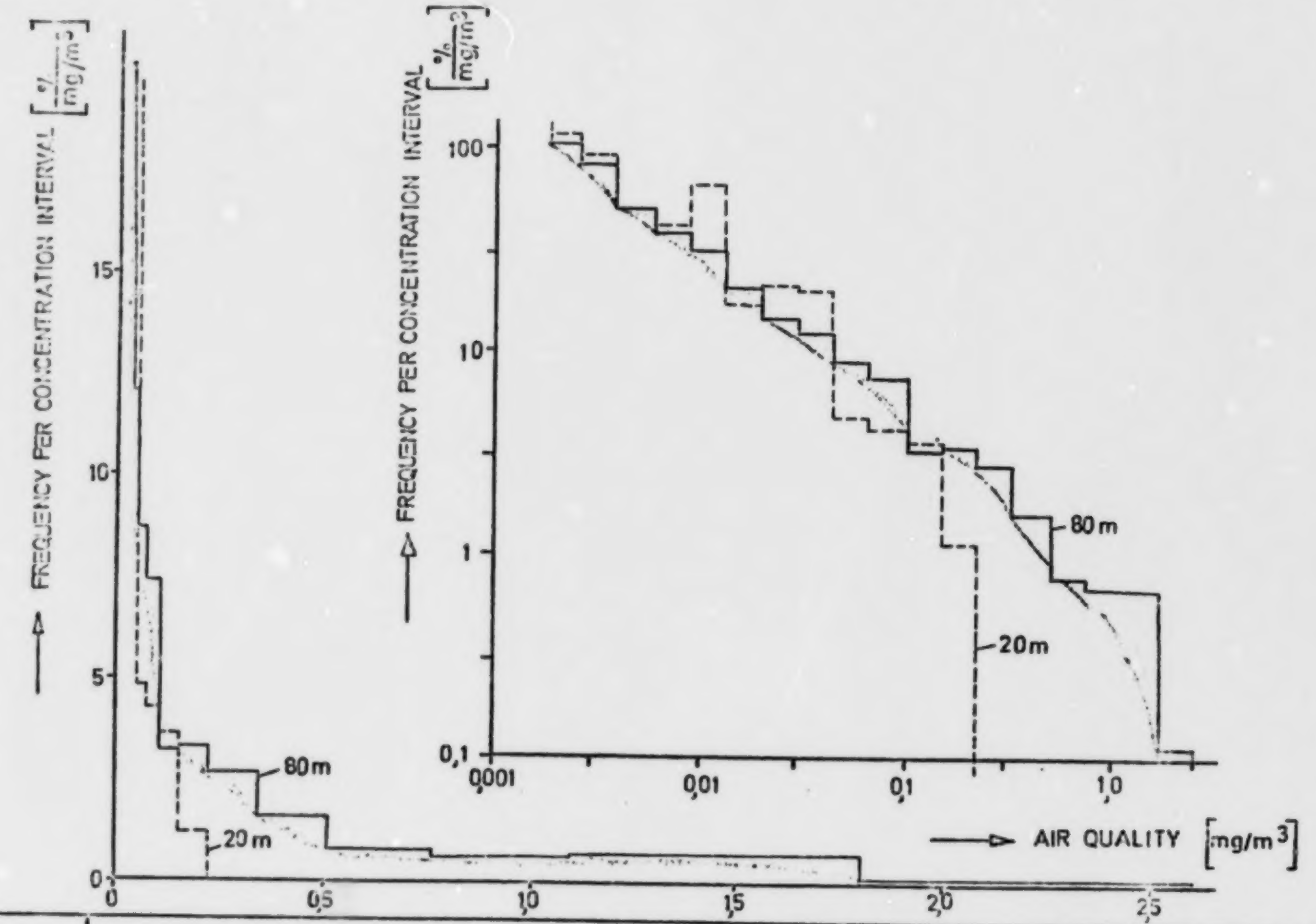
Bild 32: Immissionen Kohlenmonoxid. Schnitt entlang angenommener Windrichtung

During the discussion the kind of display of statistical distributions calculated was asked. As an example the following figs. may serve. Here the expected excess frequency depending on concentration is shown for a point calculated in the vicinity of 3 sources of about 40 m height using the weather situation distribution of Cologne.



Excess frequency of expected air quality at different heights in a distance of 500 m from a sct of 3 sources

731



Frequency of expected air quality at different heights in a distance of 500m from a set of 3 sources

7311

Chapter XIII

THE REGIONAL AIR POLLUTION STUDY - UPDATED

by

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I. Introduction

At the last meeting of the NATO/CCMS Expert Panel on Air Pollution Modeling, McCormick[1] presented the plans for the U.S. Environmental Protection Agency's Regional Air Pollution Study (RAPS). In the present paper we will briefly present updated plans for the scientific work to be undertaken in association with RAPS, and we will describe the Regional Air Measurement System (RAMS) currently being implemented in St. Louis to collect the data required for RAPS. Since a primary purpose of RAPS is to develop valid models of urban air quality we will present a suggestion as to how we might proceed with this modeling. Finally we will briefly outline a new comprehensive urban scale model (WATPC) under development in our laboratory. It is anticipated that this will be the primary component of the RAPS model.

II. Objectives of the Study

The overall objective of the Regional Air Pollution Study is the development of mathematical simulation models of air pollution processes. The models will be quantitative formulations of all the atmospheric processes affecting pollutants, i.e., dissipation of pollutants by diffusion, advection and other transport processes, transformation of pollutants by chemical reactions, and removal of pollutants. A tool of this sort would allow prediction of the utility of pollutant control actions and strategies. If the models are accurate and the data input correctly known or forecast, their output will show the effects of changes within the region, whether these effects are a result of controls or are inadvertent. The accuracy of the models will depend on the degree to which the atmospheric processes are understood and describable using mathematical techniques.

Although the objective of the study can be stated in a few words, the problems to be encountered in seeking the objective appear to be exceedingly complex and wide ranging. The study will require investigations in meteorology, atmospheric chemistry, aerosol physics, applied mathematics, and other disciplines. Some of the steps in the investigation are listed below.

(1) Evaluate the capability of current and proposed mathematical simulation models to describe the transport, diffusion, and concentration of both inert and reactive pollutants over a regional area.

(2) Develop a more complete understanding of the atmospheric motions over an urban region, both those imposed by the presence of urban structures, heat sources, and pollution, and those naturally present in the atmosphere that influence the concentrations of pollutants on an urban scale.

(3) Develop a more complete understanding of the system of chemical transformations, gas-particle interactions, and photochemical processes that take place in the urban atmosphere.

(4) Determine the correct rate-constants for use in the systems of chemical rate equations for different ambient atmospheric conditions.

(5) Test the evolution of the models in laboratory experiments and in field experiments.

(6) Evaluate factors of significance to the design of improved control strategies in the urban/rural complex, including economic costs and the roles of land use and community planning.

An important outgrowth of the regional study will be the development of an improved technology that can be applied in local and regional control operations. Most noteworthy will be the techniques that must be developed in order to describe adequately the emission inventories of both stationary and mobile sources. The study is expected also to push forward the states of the art in air quality and meteorological monitoring, data handling, and data analysis. The complete RAPS model might be oriented around a main driving module which calculates the wind structure and thermal structure on a grid placed over the urban area. A whole class of submodels for emissions, pollutant transport and diffusion, transformation (HC, NO_x, SO_x models), aerosol generation and removal processes can then be added onto the fundamental meteorological module.

The application of air quality models is only in its early stages. Widely diverse models exist and others are continuously being developed. These models cover a range, from quite limited problems, such as diffusion from a single point source, to the extended scale covering large urban complexes. Turner and Lee,[2] in a paper of these proceedings, have listed a number of current air quality models. Only in a few simple cases, however, are the models sufficiently tried and verified to warrant confidence in their use.

There are many reasons for this state of affairs. The major reason is that research has not been undertaken on an adequate scale. Wich the limited funds and resources available to date, progress has lagged far behind the need. The development and verification of suitable models are also very difficult problems, especially on the urban scale, which depend strongly on the availability of adequate data on which to base the formulation. It is possibly even more difficult to assess the model capability and measure its precision accurately, especially where long time-periods are needed to provide an adequate basis of comparison. Operation of models, for both description and prediction, has generally been constrained, and the evaluation of results against observations has frequently been inconclusive.

A decisive limitation in the model development process lies in the difficulty of observing a sufficiently broad set of conditions. This area is fundamental to all aspects of the problem, and its shortcomings cripple every subsequent endeavor. Thus, many existing models are based on very limited data sets that have been acquired routinely for quite different purposes, e.g., air-way weather observations, and are woefully inadequate in both extent and spatial and temporal resolution for the development and verification of models.

The lack of the basic data results from the high cost of collecting such data, on sufficiently continuous and extensive scales in space and time. When attempts have been made to set up special networks of observational facilities and carry out intensive data collection programs, the results have often left much to be desired and have reflected the shortcuts that had to be taken because of costs of instrumentation, and in collecting and handling the data.

Even with the emergence of relatively moderately priced automatic data processing facilities, the acquisition of basic data remains a considerable and costly undertaking. But to those considering the problems of air quality management, it has become increasingly clear that little progress can be made in the solution of such problems unless they are treated on a major and extended scale.

The difficulties of air quality management are apparent in the context of Air Quality Regions, where emissions within the region are to be related to air quality standards. For these purposes it is necessary that at all scales, from the local to the extended regional scale, there is an adequate understanding of how emissions from the several sources combine and react to produce concentrations of specific pollutants through the area. This is particularly the case where the air quality of large rural and suburban areas is greatly affected by emissions from urban centers that may be up to 100 miles away. Control and abatement procedures must take these indirect effects into account. To formulate economical and realistic strategies for such procedures, however, it is necessary to consider the less direct aspects of health, economics, land use, and community planning in the urban/rural complex.

In the application of simulation models to decisions on control strategies, it is most urgent to ensure that all concerned have confidence in the approach. There are large financial involvements; the livelihood of whole communities may be at stake, and there may be tremendous pressures on limited resources to plan, implement, and enforce control strategies. Sound modeling capability, having demonstrated accurate results, would serve all aspects of these interests and would provide the basis on which sound enforcement strategies may be sustained.

The Research Plan - In order to achieve the objectives of RAPS a continuous monitoring network will be established. The precise details of how this network will be used are discussed in the RAPS study plan which has been disseminated in preliminary (draft) form. This plan is designed to advance the existing state of knowledge in air pollution on a broad front. In outline the general areas of research are:

100 Series -- Emission Inventory
  101 Stationary Source Inventory
  102 Mobile Source Inventory

200 Series -- Atmospheric Transformations
  201 Pollution Distribution
  202 Aerosol Studies
  203 Kinetics Submodels
  204 Transformations of Point Source Emission
  205 Spatially Averaged Pollutant Measurement
  206 X-Ray Fluorescence Measurements of Metals
  207 Gas Chromatography-Infrared Spectroscopy of Trace Substances
  208 Photolysis Rate of NO_2
  209 Particle Measuring Systems
  210 Gas Measuring Systems

300 Series -- Atmospheric Structure and Dispersion
  301 Climatology
  302 Energy Balance Studies
  303 Boundary Layer Structure
  304 Tracer Studies
  305 Pollutant Variability

400 Series -- Removal Processes
  401 Precipitation Removal
  402 Surface Scavenging of Pollutants

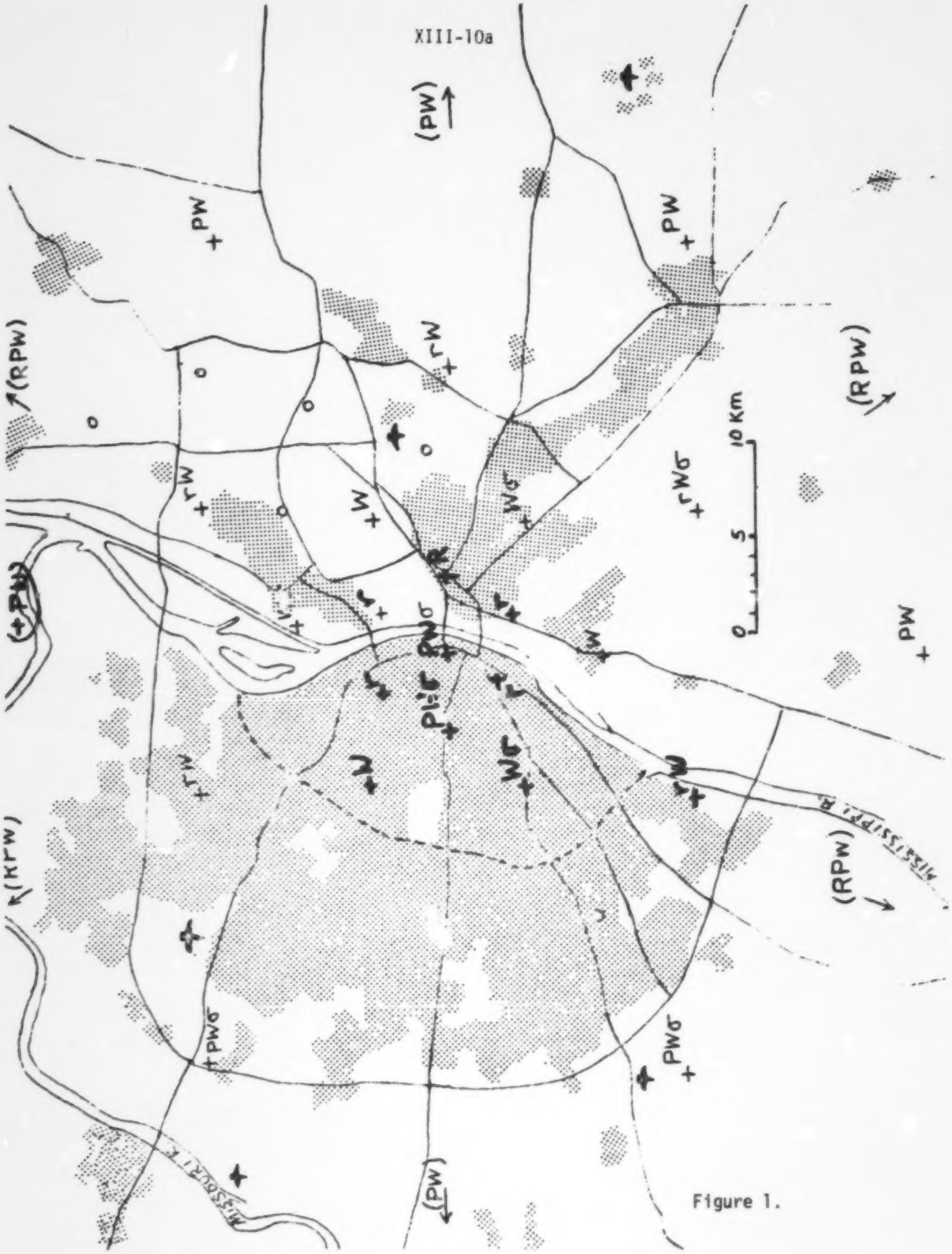
We have deleted from the formal Research Plan the Mathematical Simulation Section since these simulations will be closely related to the entire plan and will be so represented subsequently. The control economics section, while no doubt an extremely significant portion of the overall study, has also been deleted here. Further details of the Research Plan are presented in the RAPS Study Plan.[3]

The research will be done using the continuous recording network (RAMS) supplemented with excursionary research projects that have rather specific purposes. The requirements of the monitoring system were developed after numerous discussions between the various disciplines involved in the study, and consideration of the appropriate monitoring constraints. The instrumentation will provide a general baseline of information. Additional information, and particularly regarding the meteorology and the aerosol characteristics of St. Louis, will be available on a casual basis from the METROMEX study of urban influences in geophysical processes.[4]

III. The Regional Air Monitoring System

Since the major purpose of RAPS is the development of valid models of air quality it is necessary to collect a large body of statistical data simply to ensure that a large number of possible situations have occurred and have been recorded. Since many different chemical species are of concern, some of which are not easily measured, the network must include some expensive state-of-the-art instrumentation. To satisfy these needs a network of air quality and meteorological instrument stations will be established, within an area roughly enclosed by a circle of 30 km radius from the Gateway Arch, St. Louis, Mo., as its center. A central support facility will be provided, for automatic and manual data handling and processing. The RAMS stations are expected to be linked to the central facility by telephone circuits for automated data recording. Other components of the St. Louis Facility for field studies will include mobile monitoring stations, mobile laboratories, atmospheric sounding stations, helicopter and aircraft instrument platforms, and miscellaneous other measurement capabilities.

The sampling station areal density will be roughly proportional to the gradients of long-term mean concentrations (seasonal or annual). Shorter-term gradients will be measured by the portable instrumentation. In addition, an attempt will be made to provide with the network, a reasonably complete set of source-receptor relationships. Previous studies provided some information on patterns of SO_2 and suspended particulate concentrations calculated from diffusion models.[5] These indicate that the main spatial variations are limited to a radius of about 15 km, centered in downtown St. Louis. More limited information is available concerning the distribution of automotive pollutants. For the primary pollutants, modeling studies indicate that spatial variations of concentrations are quite highly


(PW)
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MISSISSIPPI R.
MISSOURI R.

Figure 1.

correlated with spatial variations of emissions, and thus, in a restricted sense, to "urbanization." (The significant street-scale variations are here being ignored.) Concentrations of secondary pollutants are expected to show a much lesser degree of fine-scale variability, with the distribution being a broad plume, having a width about that of the urban area, and extending downwind. Based on the criteria and inferences concerning the distribution of pollutants, the highest station density should be centered over the downtown area, with station density decreasing with distance.

The network shown by Figure 1 follows from the above criteria and the constraints of available funds. It consists of a central station, located in the vicinity of the Gateway Arch, with four concentric rings of six stations each (indicated by X's in Figure 1) at distances of 4, 8, 15, and 30 km from the central site. At each of these 25 stations the following pollutant concentrations and meteorological parameters will be measured: Carbon monoxide, methane, total hydrocarbons, hydrogen sulfide, sulfur dioxide, ozone, nitrous oxide, nitrogen dioxide, fine particulates; wind speed and direction, ambient temperature, and dew point temperature.

Additional sampling sites would be chosen in the northeast sector to sample in the area of the expected maximum impact of the large sources on the Illinois side of the river, when winds are from the southern sector; these stations are indicated by circles, but the best array will be determined from a more specific survey of locations of the major point sources. The pollutants to be sampled at these locations will depend on what the sources emit. One or two additional sites in the southwest quadrant (indicated by the single circle on the figure) may be desirable to adequately sample the build-up of automotive pollutants across the rural-suburban-urban fetch with southwest winds.

The supplementary meteorological measurements to be made at the various sites are indicated by the letters in the figure. At four distant sites and two urban sites, comprehensive solar and sky radiation measurements (R) are to be made. These will be supplemented by pyranometer measurements (r) at the 4- and 15-km sites. Pressure measurements (P) will be made at the central site and selected outer stations. Horizontal wind components (W) will be measured at all sites of the regular array, except where a representative exposure is impractical. At eight of the wind sites, the vertical wind component will also be measured, and the variances (σ) of all three wind components will be obtained. If two suitable tall towers can be located and installation of equipment is possible, temperature and temperature differences between levels will be measured, as well as the three wind components and their variances. There are no suitable towers in the main urban area, but some may be found in the 15-30 km range from downtown.

The horizontal distribution of pollutants at or near ground level is only a portion of the information needed on transport and transformation. Most atmospheric motion is horizontal but the wind direction and speed, air turbulence, and pollutant characteristics and concentrations, all vary with height above the surface. Day to day variation occurs in the maximum heights to which pollutants rise and are transported. It is therefore important that vertical soundings of essential atmospheric parameters be made on a regular and frequent schedule.

Current plans call for a network of three or more stations that will make regular soundings of wind, temperature, humidity and pressure, at six-hour intervals and more frequently on selected days. The station locations will be separated by at least 25 km, bracketing the central urban area. Soundings will be recorded to 3,050 m. or the height of the mixing layer, if higher than that. Regular helicopter or aircraft sounding will be made, weather permitting, for the collection of air quality information. It is intended that such soundings be made at several locations around the St. Louis area and up through the layer of mixing. The data from the fixed monitoring network will be telemetered to a central computer facility which will control the network operation, and clean and store the information.

All data will be automatically identified. This will permit the addition of data from other sources. It is currently planned to add all RAPS information including sounding, aircraft data, tracer data, chemical and ecological sample analyses, when available, to a common data bank.

IV. The RAPS Model System

A great deal of modeling and many models will certainly result from the RAPS study. These will no doubt range from the "hard" scientific variety described herein, to a somewhat "softer" total ecosystem model, that considers such parameters as the total incoming energy and the partitioning of the energy outflow, or finally, to a so-called decision model for cost-benefit analysis.

In the discussion that follows we shall be concerned only with the modeling that is directly related to the EPA missions to maintain air quality. Even with this limitation a great diversity currently exists in scientific models of air quality, and the need for a single organizational model is easily justified.

In recent years, a number of urban air quality models have been developed.[6] A few of these have attempted to consider the inclusion of a calculated wind field [7-10] but none so far has achieved a successful coupling of air quality modeling with meteorological modeling. In general it has been common to consider the wind field either as uniform across the entire urban area[2,11] or generated by an interpolation from a few surface stations.[12,13] In certain cases some of the more sophisticated models have required an extensive hand analysis of the flow field.[14] However, on the basis of current experience and the apparent direction of future modeling activities, it seems that the inclusion of a proper flow field will become more and more critical as air quality models take on more realistic tasks. While the efficiency of the computer suggests that numerical modeling is the only way to proceed in order to obtain valid three dimensional flow structure over an urban area, the specific fashion in which this objective might be achieved must be determined. There are approaches ranging from a machine produced "objective" analysis of the surface observations (in its simplest case $1/r^2$ interpolation of data), to a dynamically predictive solution of the appropriate equations, given proper initial and boundary conditions. Of course, there are a variety of mixes allowed between these two extremes. The advantages of objective analysis are simplicity, speed and a relatively short development time. The results, however, are rather limited to specific locations for which sufficient data are available both for verification and for routine operation. Since most urban areas cannot provide this information an objective of the research will be to ascertain the minimum observations required to perform a reasonable objective analysis.

An urban model must have the capability of determining the concentrations of a number of characteristically different pollutants. As an example, CO is emitted from ground level sources and must disperse into a substantially different environment than would, say SO_2, emitted from a tall stack. A simplified meteorological analysis nevertheless might provide exactly the same atmospheric structure as input to both of these models. However, even with meteorological measurements at 25 stations over the city, as the RAMS will provide, it is likely that certain characteristic motions, say, in a scale from 1-10 km, will not be observed. In fact the only way to really illucidate the details of the flow structure over a city is with an accurate dynamical model. It is clear then that any realistic RAPS model will need to consider so many pollutants and in such fine detail that good fluid-field data are an indispensable and inseparable part of the model. However, it must be noted that a model of sufficient magnitude and detail to correctly handle RAPS will be a research objective in urban meteorology for many years. For this reason we will be forced to compromise to produce a working RAPS model in the next two years. This, viewed in proper perspective, will be an interim model that needs to be continuously developed and improved.

The RAPS model suggested herein is organized around a calculation of the wind and temperature field. It often appears that the only unifying principle of urban air pollution is, that it occurs in the air (or on the air's interfaces) and in places different from where it was released, because of the air motions. If one can model where the air goes, it is a relatively easy matter to model where various encaptured contaminants will go. In the presence of photochemical and other chemical activity it is equally important to model where the air goes, since the input material is changing, depending upon what meteorological conditions it encounters (i.e. solar radiation, precipitation, etc.) along its particular trajectory, and the extent to which material is removed by depositional processes. Hence, it seems obvious that the first step in producing a RAPS model must be to develop a wind and temperature structure model. To put these concepts on a firmer basis we have outlined a preliminary rationale for the RAPS model system. A somewhat uneven outline touching on some of the main points of this rationale is given below.

1. Main Meteorological Module

The main organizational element of the RAPS model will be a calculation of wind and temperature structure over the St. Louis area. Three distinctly different mechanisms for approaching this are suggested:

(a) Refined objective analysis -- machine organization and usage of data taken by the RAMS (completely diagnostic).

(b) Highly parameterized model -- a vertically integrated (2 layer or so) dynamic model perhaps coupled with an energy balance calculation.

(c) WATPC -- a fully three dimensional-dynamic predictive model including turbulent transfer and surface energy parameterization.

2. Air Quality Submodels

These can be many in number since the only difference between current state-of-the-art and what would be used for a RAPS model is a compatibility with (a), (b), and (c) of 1 above.

(a) Inert pollutants

(i) CO -- existing model for CO (SRI)[11] could easily be incorporated into any of the models suggested by 1. We would propose development of a grid point calculation of CO in order to present city-wide patterns at selected times.*

(ii) SO_2 and particulates -- existing models calculate SO_2 concentrations for given trajectories. Development of a grid point SO_2 model is underway. Incorporation of transformation mechanisms would be considered eventually.

(b) Ozone Photochemical Pollutants

(i) Complex Photochemical Models -- under contract SAI[14] is improving upon existing Los Angeles models and extending some to St. Louis.

(ii) Parcel Models -- many of the more complex photochemical models are trajectory-oriented.[12,13] Any of these could be used as such by adaptations as described in 2(a)(i).

*This statement applies to all of the trajectory-oriented sub-models.

(iii) Maximum Reduction Models -- it should be determined what the maximum meaningful simplification is for the calculation of ground level NO, NO_2, O_3.

(iv) Process Models for Photochemistry -- the models above cannot be satisfactory for the purpose of studying photochemical processes. Thus we propose that this disciplinary task be taken on by the photochemists themselves. Certainly, however, the development of (iii), which might be considered a RAPS final objective, could not go forward without cognizance of and continuous iteration with (iv).

(c) Aerosol Models

(i) Sulfates -- sulfate aerosol, generated ultimately from SO_2 released from stationary sources, could be modeled by similar techniques, among others, to those employed in ozone photochemistry. The problem is currently under study. We would suggest a simple model consisting of perhaps SO_2, NH_3 and H_2O concentrations.

(ii) Smog -- small aerosols generated by conversion of automobile exhaust can be modeled by assuming a simple auto-conversion mechanism not unlike that used in cloud modeling. Preliminary work has been done on a trajectory oriented parcel model. An approach like this could easily be refined and incorporated into the RAPS model.

(iii) Process Models for Aerosols -- similar to (b)(iv) one would anticipate the development of a comprehensive set of aerosol dynamics models.

3. Removal Processes

In general there are two types of removal processes to be modeled, namely, those which occur because of the water vapor present in the atmosphere, and those which occur because of surface impingement.

(a) Precipitation Removal

Two fundamentally different mechanisms accounting for precipitation removal, are washout, which is essentially a collision process involving the collection of aerosol by falling precipitation and rainout, which is essentially a cloud microphysical process involving the pollutant in the cloud condensation nuclei.

(i) Parameterization model -- A simple attempt to incorporate precipitation removal between the main meteorological module and the AQS's would be to simply reduce the concentration aloft of the appropriate species according to calculated meteorological information, and increase the amount of pollutant in the lower levels which would in turn be presented to a scavenging model. Certainly much data will be required to validate such an approximation.

(ii) Cloud Microphysical Model -- A number of cloud models exist in meteorology which are capable of simulating the cloud development process from the initial CCN spectral distribution to a full blown cloud system. This will be under study and development by METROMEX, and a final result should be able to interact with WATPC.

(b) Surface scavenging

Removal processes associated with surfaces are as diverse as (a) the surface being dealt with, i.e., organic, non organic, solid, liquid, etc. (b) the geometric orientation of the surface and (c) the size of aerosols of concern, which might range over a number of orders of magnitude. Any modeling must be highly parameterized. One can successfully parameterize the physical processes involved based upon such concepts as fall velocity, turbulent diffusion and even molecular forces, but the prospects for such parameterization on biological surfaces are less hopeful.

(i) Deposition velocity model -- A simple parameterization of the scavenging process is to relate the mass rate of change of a pollutant near a surface to its ambient concentration by defining a pseudo-velocity to account for any removal. The deposition velocity so defined is mainly a function of surface type.

(ii) Process models for deposition -- As in other sections one might envisage detailed microphysical and biological models of surface capture.

4. Emissions

Emissions inventories will never be available in the required resolution for all modeling applications. Emissions models therefore will be required to reduce the average or total emissions to the rather fine temporal and perhaps spatial scales that are needed.

(a) Stationary Sources

"Models" exist for converting, either fuel input to a source, or product output from a source, into an emission profile. The inputs or outputs are broken down on an annual basis or at best a seasonal basis. For specific sources it might be possible to determine the most important parameters accounting for variability on the hourly, daily and weekly time scales, (daylight or not, holiday or not, climatology, etc.) and develop models incorporating these parameters to calculate fine-scale emissions information.

(b) Mobile Sources

Models can be developed to convert from emissions per vehicle-mile to total emissions, by considering the traffic mix and density as a function of time, as well as the highway distribution.

The modeling plan is a comprehensive undertaking on a scale never before considered in air quality simulation. It is nevertheless warranted on the basis of the data that will be forthcoming from RAPS. We will need to rely on the assistance and criticism of a great many environmental scientists. Hopefully a major scientific objective of RAPS will be to seek some generality from the chaos which is apparent in the urban environment today. A model allows a common ground for communication among scientists with different backgrounds, and provides a forcing to communication that would not necessarily otherwise occur.

V. WATPC

In order to meaningfully calculate the wind and temperature fields in an urban area, or other complex meteorological situation, for the wide range of conditions that are of interest in air quality applications, a rather sophisticated numerical model is being developed by the Model Development Branch, of the EPA Meteorological Laboratory. In earlier sections of this paper we have outlined the needs and state-of-the-art in air quality modeling. In a separate paper[15] questions of the appropriate scales, the degree of predictability expected and the general approach are investigated.

Here we will present the Wind and Temperature Predictive Code (WATPC) in its simplest form.

WATPC is a three dimensional dynamic prediction of the wind and temperature fields over an area of about 30 x 30 x 3 kilometers with a resolution of 1 x 1 x .2 km. The one kilometer resolution is rather fixed. Our feelings are that meaningful meteorological field modeling on scales much smaller than one to two kilometers is virtually impossible, if one also wants to consider some of the significant urban scales and mesoscale interactions which drive the urban circulation. The wind tunnel and water channel provide excellent facilities for studying problems of scale smaller than 2 kilometers. The 200 meter uniform vertical resolution currently being used is not as much of a restriction as the horizontal scale (because of the manner in which the calculation is programmed) and certain improvements will be included eventually which will allow for better resolution in areas of significant vertical structure.

The basis of WATPC is a solution of the three motion equations for $\underline{V} = (u, v, w)$ the wind vector, with similar equations for the temperature and a calculation of the pressure field. It is emphasized here that we do not assume the large scale meteorological balance between pressure and gravity (hydrostatic distribution) that is often inappropriately suggested to be applicable for the problem.

The equations, within the Boussinesq approximation, for dry atmospheric motion can be written in general form

$$\frac{d}{dt}\underline{V} = \underline{B} - \frac{1}{\rho}\nabla p + \nabla : \underline{\underline{T}} - \underline{f} \times \underline{V}$$

$$\nabla \cdot \underline{V} = 0$$

$$\frac{d}{dt}\Theta = \nabla \cdot \underline{D} + S$$

where $\frac{d}{dt}\langle\cdot\rangle = \frac{\partial}{\partial t}\langle\cdot\rangle + \underline{V} \cdot \nabla\langle\cdot\rangle$

$\underline{V}$ = (u, v, w) = three dimensional velocity field

B = $\left(\frac{\Theta - \Theta_0}{\Theta_0}\right) g \underline{k}$ = buoyancy force

ρ = density

P = pressure deviation from hydrostatic

$\underline{f} = f\,\underline{k}$ = Coriolis parameter (vertical component of the earth's vorticity).

$\underline{\underline{T}}$ and $\underline{D}$ are the stress tensor and temperature flux vector respectively. Since the motions being simulated are fully turbulent, the dependent variables represent mean values, while the stress tensor and flux vector represent Reynolds stresses and turbulent fluxes, but neglect molecular terms. A primary consideration is how one goes about parameterizing such terms.[16] A number of schemes will be considered, although our preliminary model simply uses conventional eddy viscosity and eddy diffusivity ideas. Thus presently we have

$$\nabla : \underline{\underline{T}} = K_H \left(\frac{\partial^2}{\partial x^2} \underline{V} + \frac{\partial^2}{\partial y^2} \underline{V} \right) + K_W \frac{\partial^2}{\partial z^2} \underline{V}$$

$$\nabla \cdot \underline{D} = K_\Theta \nabla^2 \Theta$$

where K_H is a horizontal eddy diffusion coefficient, K_W is a vertical diffusion coefficient and K_Θ is the thermal eddy diffusivity. It should be emphasized that a small-scale turbulent flow model of this resolution will of necessity have substantial transfer of energy between the smallest scales of resolution. A simple eddy viscosity is most likely not appropriate as a parameterization of these transfers. Our first improvement will be to consider an eddy viscosity dependent upon local flow structure, say proportional to the grid resolution and the mean deformation of the fluid.[16] However, in order to correctly represent the fine scales, it will probably be necessary to consider at least a two-equation model of the turbulence. One model might be a predictive equation derived for the turbulent kinetic energy, and one for the turbulent energy dissipation. A great many approaches to this problem are evolving rather rapidly at the present time and the proper way to parameterize the undetermined terms in these equations for E and ϵ is still somewhat open.

A second primary concern must be with the various boundary conditions required by the model. Horizontal boundary conditions should, of course, be time variable. They will be determined eventually from a supergrid-scale, mesoscale meteorological model. From a mechanistic viewpoint the horizontal conditions need to allow free flow into and out of the computed volume and hence the derivation of velocity components are set to zero. The meshing of models of different scales is a very difficult task and one which will require some significant research to perform successfully. However, one of our prime interests is in calculating the flow field when the ambient winds are light so that the supergrid flow does not overly influence the urban flow. These cases, of course, are of primary interest in air pollution. In this situation the flow is predominantly determined locally by thermal and mechanical forcing. Thus one must pay special attention to the boundary conditions imposed at the bottom of the model. The actual building height variability is averaged across grid areas to produce a mean building elevation. The horizontal flow at the lowest grid level is then either zero, if the mean building height is higher than the grid point, or calculated by assuming a logarithmic surface layer between the mean building height and the grid level, when the latter is lower than the first grid point.

The thermal boundary conditions are not nearly so easily dealt with. Our feelings are that these are the primary forcing functions in urban scale flows and as such they must be well treated. Our model will be coupled with a somewhat sophisticated surface energy budget calculation being developed by E. C. Nickerson.[17] The two forcing inputs to this energy budget model are the incoming solar radiation and the wind field. The primary component of this budget is the heat storage capacity of the surface. Since urban surface structure is very different we expect again to average over actual surfaces to arrive at some type of mean storage coefficient. This will certainly vary from grid area to grid area, probably most strongly as a function of land usage.

The mechanics of the numerical approximations are described in a number of publications[16,18] and will not be dwelt upon here. Suffice it to say that the velocity and temperature are calculated by marching forward in time while pressure is calculated by inverting an elliptic equation, formed by taking the divergence of the motion equations and enforcing the incompressibility condition. The inversion is done each time step, by an iteration scheme which incorporates a solution of the two-point boundary value problem in the vertical.

VI. Summary

This paper is an attempt to provide a brief summary of some of the research associated with the EPA-RAPS. We hope that RAPS will have a synergistic effect on environmental science, such that five years from now these research objectives will be out of date.

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Chapter XIV

Users' Needs
and the
Applications
of
Air Quality
Simulation Models

by

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Prepared for the 4th Meeting of the Panel on Modeling of the NATO Committee on the Challenges of Modern Society

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USERS' NEEDS AND THE APPLICATIONS OF AIR QUALITY SIMULATION MODELS

by

D. Bruce Turner and Russell F. Lee

Introduction

There is a wide variety of users and potential users of Air Quality Simulation Models in the United States. Starting with the Environmental Protection Agency, there are two main groups working in the air pollution field that have the need for models. First are the technical personnel who are concerned with the abatement of air pollution and the meeting of ambient air quality standards. A second and largely administrative group comprises those responsible for the formulation of policy and the impact of legislation and proposed rules upon air quality. A third group, concerned primarily with ecological problems and the interactions of air pollution, water pollution, and solid waste, also has a need for air quality simulation models.

There are also other users in the federal government besides the Environmental Protection Agency. Notable is the Atomic Energy Commission who has played a lead role in the study of dispersion from point sources (Slade, 1968; Gifford, 1961; Briggs, 1971A, 1971B) and from urban sources (Gifford and Hanna, 1970; Gifford and Hanna, 1973; Hanna, 1971) as part of their reactor safety program. The Federal Highway Administration and the Federal Aviation Administration, both in the Department of Transportation, are also interested in estimating the impact of proposed facilities that are under their supervision. Another large body of potential users of models comprises the state and local air pollution control agencies and the state and regional planning authorities and their consultants. A final group of users are air pollution consultants and engineering firms.

Current federal regulations and legislation have a profound effect on the need for models. National ambient air quality standards have been set for a number of pollutants. These standards generally are expressed in the form of a mean annual concentration and a maximum concentration not to be exceeded more than once per year. These short term standards are generally for averaging times on the order of 3 to 24 hours. It is therefore desirable to have air quality simulation models capable of estimating concentrations annually and also for short time periods of a few hours.

The National Environmental Policy Act, signed January 1, 1970, requires each federal agency to prepare a statement of environmental impact in advance of each major action, recommendation, or report on legislation that may significantly affect the quality of the human environment. Each statement must assess in detail the potential environmental impact of a proposed action, and all federal agencies are required to prepare statements for matters under their jurisdiction. Such actions may include new highway construction, harbor dredging or filling, nuclear power plant construction, large scale aerial pesticide spraying, river channeling, new jet runways, munitions disposal, bridge construction and others. Because of the variety of sources to be considered, a number of air quality simulation models are required to determine impact upon air quality.

In connection with ambient air quality standards, the states are required to furnish implementation plans indicating how they intend to meet these ambient air quality standards. These plans must primarily consider the regional scale.

Stable Pollutants from Isolated Point Sources

One of the users' needs is for a model to estimate concentrations from isolated point sources, of the more stable pollutants such as carbon monoxide, suspended particulate matter, and sulfur dioxide. This modeling ability is needed by EPA in order to review impact statements and to provide technical assistance to the states. It is also needed by the states and local control agencies with regard to permit applications. Finally, it is needed by engineering firms and consultants in the design of point sources. Point source steady-state Gaussian models based on the equations and dispersion parameters of Pasquill (1961) and Gifford (1961) have been used to make such estimates. These models are most reliable for level or gently rolling terrain and for short time periods on the order of 10 minutes to an hour. They are also quite reliable for elevated releases with stack heights up to about 100 meters and with reduced reliability for greater heights. In applying these elevated point-source models, the effective height of the plume is usually found using the methods of Briggs (1971a, 1971b). For higher sources, complications occur due to wind speed and stability variation with height. For source heights above 100 meters, the Tennessee Valley Authority has done considerable research on dispersion that includes the determination of dispersion parameter values. They have also developed models for these source heights (TVA, 1964; TVA, 1970; Thomas et al., 1970; Carpenter, et al., 1971; Montgomery, et al., 1972; Montgomery, et al., 1973). Because the period involved in the definition of the ambient air quality standards is generally longer than one hour, it is desirable to make estimates for time periods such as 3 hours or 24 hours. In general, it is felt that these estimates can best be made by first estimating the concentration for each hour using the representative meteorological conditions and then averaging the hourly concentrations over the desired period. Attempting to estimate the maximum concentration for these averaging periods that occurs only once a year is quite difficult, as it is not readily apparent what conditions lead to these maxima. In an attempt to make such estimates we have used a model that calculates concentrations for each hour using data for an entire year, although we realize that year to year variations of the maximum could be considerable. Concentrations are averaged for each 24 hour period, midnight to midnight, and the maximum value determined for the whole year. Concentrations are estimated at a number of receptor points; we have used five different distances and 36 directions corresponding to each 10°. This particular model can be used to estimate concentrations from a single plant with multiple stacks, although it is not suitable when a number of plants are located in the same general vicinity. Since ambient air quality standards must be met by considering concentrations resulting from all sources, and not just a single plant, it is necessary to consider the total source distribution. One multiple point source model does this by performing calculations for any number of point sources and selected receptor locations. All of these point source models are primarily applicable to relatively stable pollutants such as sulfur dioxide, suspended particulate matter, and carbon monoxide.

There is also a need to estimate concentrations from point sources in areas of complex topography. For this situation the steady-state Gaussian plume models are not adequate, especially if the terrain features extend above the centerline of the plume. Physical modeling using wind tunnels or water channels (Snyder, 1972) will help in the understanding of the wind flow.

Numerical modeling is also being attempted for sources in complex terrain. Some of the approaches utilize numerical meteorological model based on the topography and measured meteorological parameters to determine the flow field, and then use this as input to a dispersion model to determine the concentrations. Two cases where it has recently been desirable to estimate concentrations from point sources in complex terrain relate to large coal fired power plants and smelters located in mountainous terrain.

Other uses of point-source models include the preparation and review of impact statements, the design of control systems and stacks, and the review of permit applications. Users currently include the federal and state governments, industry, and many consultants.

Stable Pollutants from Multiple Sources

For estimation of concentrations of air pollutants in urban areas we need to turn to multiple source models. Frequently this is accomplished by considering two classifications of sources: significant point sources, and then all other sources lumped together as area sources. For the longer period averages, such as seasonal or annual concentrations, the AQDM (TRW Systems Group, 1969), or the more recently formulated CDM (Calder, 1971), are applicable when no significant terrain features are influencing the air flow. Both of these models express emission information for point and area sources as either annual or seasonal means and accept stability wind rose information. Calculations are then performed by wind sector.

For shorter averaging times (1 hour up to 24 hours) and when a definite flow of air occurs so that a single mean wind direction can be chosen for each hour that is representative of the entire urban area, steady-state Gaussian models have been used. In most cases the dispersion parameter values have been modified from those used in open areas, so as to include effects of the greater urban surface roughness. Consideration of only the area emissions directly upwind from the receptor, commonly called the narrow plume hypothesis, can be used (Calder, 1971 and Hannah, 1971). Although short term models of this type have been in existence for some time, few have been documented to the extent that they are readily usable. Under contract to EPA, Geomet, Inc. of Rockville, Maryland is documenting a short term model called SCIM (Sampled Chronological Input Model). This model calculates frequency distributions of concentration at a receptor by performing calculations for a sampling of 1-hour periods, selected from the total period that is of interest.

Another short term model called RAM, for Real-time Air-quality-simulation Model, is being developed for short time calculations of 1-hour up to 24-hours. This model is also a steady-state Gaussian type model only applicable to relatively stable pollutants. Calculations are made for both point and area sources. This model is an attempt to permit rapid calculation and for a minimum of receptor points. Emissions for both point and area sources are included.

The more significant of these sources is determined and then the locations of receptor points at points of maximum concentration downwind from these significant sources are calculated. In addition to the locations of maximum concentration, other receptor locations may be specified arbitrarily. An option is available on the computer program to augment the receptor points from the above two categories by an evenly distributed hexagonal array of additional points. The distance of spacing between stations is selected by the user. Also points in this array are not added if one of the specified or calculated receptor points is within a specified distance of the given location. This keeps the number of receptor points to a minimum and the ones that are used are at locations where the concentration is expected to be highest. This model was designed primarily for real time use, such as making estimates of 24 hour average concentration 6 hours from now. For such a case, actual meteorological measurements would be used up to the present time, and forecast conditions used for the remaining 6 hours of the period. The model is limited to conditions when there is a definite flow of wind over the area and only one representative wind direction, wind speed, and stability can be used in the model.

For such a model to be applicable on a real-time basis for urban areas, a stagnation sub-model is needed to estimate concentrations under light and variable wind conditions. A sub-model for the stagnation situation is being developed at the present time. It is not now incorporated into the model. RAM is designed so that it can be used for control tactics computations. The hour-by-hour partial concentrations from the significant sources at each receptor are maintained on a tape file. If these significant sources are controllable ones, different degrees of control can be applied to determine the resulting concentrations without recalculating through the model. Thus, concentrations can be determined for several different control tactics. In addition to the possible usefulness of this model on a real-time basis to state and local air pollution control officials, it is expected to be useful to EPA groups, and to engineering and consulting firms as well, for any computations of air quality for relatively stable pollutants for time periods from 1 to 24 hours.

Both the climatological and short-term models for multiple sources are of greatest use when they estimate the concentrations from each source, or source type with equal reliability. This is desirable so that the contribution to the ambient concentrations can be properly assessed. Existing models can be used for estimating effects of various control programs and for community planning uses. They can also be used to consider the effects upon air quality of proposed legislation of proposed rule making. It is anticipated that when a stagnation sub-model becomes available it will be useful for episode control, i.e., source control-tactics. It is recognized that due to the rarity of prolonged stagnation conditions, this sub-model will be extremely difficult to validate.

Models for complex topographic situations are needed for multiple sources and urban areas as well as for point sources. Gronskei (1972) has reported good results for estimation of SO_2 concentrations from multiple sources in Oslo.

Concentrations from Mobile Sources

There is also the need to estimate pollutant concentrations resulting from transportation sources. With the two models that have been previously discussed, these emissions can be considered as area sources. In some cases it is desirable to look at the emissions in somewhat greater detail. This can be done by using line sources for highway segments. One model that will calculate short term concentrations from such sources, representative of averaging times of 1 hour or greater, and of spatial averages of something on the order of one square kilometer, is the APRAC-1A model developed under contract by Stanford Research Institute (1970, 1971, 1972A, 1972B). This model can estimate concentrations throughout an urban area by considering all of the sources in the area. The model is a Gaussian steady-state model and therefore most applicable to stable pollutants such as carbon monoxide. An addition to this model is a sub-module for determining concentrations in city street canyons. This model is useful to state control agencies in the preparation of implementation plans, and to EPA personnel required to review these plans. It is also expected to be useful to EPA in determining effects of long range strategies such as specific emission controls on automobiles. The model is also of use to urban planners for determination of general levels of air quality.

Another requirement for determining concentrations from highway segments is that of preparation of impact statements for specific highway segments. A model that can be used for estimating the effect of non-reactive pollutant emissions from highway traffic on air quality is HIWAY. This simple model does not allow for the effect of complex terrain or non-uniform wind conditions in the calculation of concentrations. Therefore it is restricted to estimation of concentrations downwind of at-grade highways on level terrain, or of concentrations downwind of a depressed highway (that is a cut section). This is a line source model with dispersion assumed to be Gaussian. Different lines are used for each lane of traffic. A trapezoidal-rule integration of point source concentrations is used in the model. This allows computation to be made for any angle of the wind with the highway, and for arbitrary locations near the highway. Concentrations from other sources are not considered in this particular model. To make estimates of concentrations from highway segments that are affected by other sources, additional estimates would have to be made for these sources and added to those determined by HIWAY. The model is most useful to those preparing and reviewing impact statements.

Another need is to determine the impact of complex sources upon air quality. These sources may consist of such things as sports arenas, shopping centers, and airports. Such sources are generally made up of a number of source types. In the case of sports arenas, the primary concern is emissions from motor vehicles. In the case of shopping centers there may also be a few point sources such as incinerators or heating plants. The airport probably represents one of the most complex source configurations in that there are emissions due to aircraft both at parking ramps, during taxiing to runways, along runways, and also on slant paths in the air during climbout or approach. In addition to aircraft emisisons there are many emissions due to motor vehicles, such as service vehicles on the aircraft portions of the airport as well as those that are used to deliver passengers and freight to the terminal. In some cases airports exist in relatively congested areas so that the emissions of air pollutants from other locations off the airport property are also of importance. For airports, a specific modeling effort has been undertaken and supported by EPA to estimate the impact of aircraft and airport emissions. For the other cases of complex sources, combinations of area and line source models should be sufficient to make estimates of concentrations. With current regulations in the U.S.A., one of the most difficult questions is determining those meteorological conditions that occur to cause the highest concentration with the frequency of once per year for averaging times of 24 hours, 8 hours, or 3 hours. Users of models for complex sources will include those preparing and reviewing impact statements. The primary intended use of the airport models is to determine the contribution from aircraft, so that aircraft emission standards can be set appropriately.

Models for Pollutants Formed in the Atmosphere

There is also a need to estimate concentrations of reactive pollutants. This includes those that we consider secondary pollutants because they are formed through the reactions of other primary pollutants. Photochemical pollutants form one of these reactive systems. Of interest here are the reactions between hydrocarbons and oxides of nitrogen to form secondary pollutants, such as ozone and oxidants. At least four different approaches to modeling photochemical pollutants have been investigated.

The fixed-cell, finite-difference models (Seinfeld et al., 1972; Eschenroeder and Martinez, 1969) calculate concentrations over a grid of cells in three dimensions, using finite-difference integration techniques to solve the classical equations of conservation of mass, including local change, advection, diffusion, reactions, and emissions. This type of model considers Eulerian or fixed coordinate cells and its advantage is that it produces urban wide concentration patterns.

Its disadvantage is that artificial diffusion or pseudo-diffusion is frequently inherent in the method as a result of the finite difference techniques that are employed. The computer time requirements for running this model are also quite large.

The moving cell models (Eschenroeder and Martinez, 1970; Wayne et al., 1971) use a LaGrangian approach, in which a moving cell or parcel is advected along a wind trajectory. One variation of this approach assumes instantaneous uniform mixing vertically within the parcel, and thus neglects vertical diffusion. Both versions neglect horizontal diffusion. The advantage to this approach is that it traces concentration history along an air trajectory. It has the disadvantage in that it is difficult to obtain urban wide patterns, and errors also occur because horizontal diffusion and convergence are not included. Computer time requirements for this model are quite modest.

The particle-in-cell model (Sklarew, 1970; Hotchkiss and Hirt, 1972) is a novel approach in which pollutant mass is represented by "particles" which are advected in accordance with an effective transport velocity that includes both the mean and the turbulent transport. Concentrations are computed according to the numbers of particles located in each cell of an Eulerian or fixed coordinate grid. An advantage to this method is that it avoids artificial or pseudo diffusion. Also it may be used to display the concentration pattern, and urban wide concentration distributions are readily seen. Large core-storage is required in the computer and the running time is large.

A fourth type of model is the multiple-box (Reiquam, 1970; McCracken et al., 1971) which utilizes an Eulerian array of well-mixed cells. These that can be quite large and variable in size so as to give spatial resolution only where needed. One version of this model does include terms for horizontal diffusion. This type of formulation is a variation of the basic finite-difference grid model mentioned above, and thus is also influenced by the artificial diffusion produced when the equations are integrated. The advantages are that the sizes and the shapes of the cells are variable so that their number can be reduced. The method only involves ordinary differential equations. The disadvantages are that it neglects vertical diffusion, and pseudo diffusion can be significant. The computer time requirements are modest.

Three of the photochemical models have been applied to a common data base of six days data for Los Angeles, California. Adjustments were made in the chemical kinetics module for three of the days in order to fit the observed oxidant concentration. The adjusted reaction rates were then used to make model predictions for the remaining three days. Results can be considered quite successful.

Recently Hanna (1973) has suggested use of a simple photochemical model. This may be quite useful for a number of applications. The primary application of photochemical models required by users is to determine secondary pollutant concentrations when emissions are significantly reduced over those of the six days' test period in 1969, that is mentioned above. It is desired to estimate the concentrations likely to occur after most vehicles on the road are equipped according to 1975 emissions standard. This implies the application of the models with emissions reduced by factors of 15 or 20. There is some doubt as to whether the lumped parameter chemical kinetics module as now incorporated in the model, will perform adequately for these greatly reduced emission levels.

Adequately validated photochemical models are also needed by those preparing and reviewing implementation plans, as well as those engaged in urban planning.

Summary

At the present time adequate models exist for stable pollutants. This is for both short averaging times, on the order of an hour to a day, and for the longer seasonal and annual averaging times. Models are available for both isolated point sources and for the multiple source situation of urban areas. However, adequate models do not exist that include complex topography, either for the point sources or for urban areas. Nor do we have adequate models for the stagnation case, where wind velocities are extremely light and winds are variable. Need also exists for models where transformation and removal processes occur, as in the formation of secondary air pollutants. For stable pollutants, models exist that will handle line-sources such as from automotively generated pollution. Research is currently underway on numerical models for the three situations: complex topography, stagnations, and reactive pollutants. It is hoped that physical modeling, through wind tunnel and water channel methods, will be useful in the solution of air quality problems where there is complex topography.

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Chapter XV

AIR QUALITY FREQUENCY DISTRIBUTIONS AND METEOROLOGY

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Abstract

AIR QUALITY FREQUENCY DISTRIBUTIONS AND METEOROLOGY

by Ralph I. Larsen, Ph.D.

Ambient air pollutant concentration frequency distributions are skewed. Various mathematical functions, especially the lognormal, have been used to describe these skewed distributions.

The cumulative frequency distributions of inverse wind speed and pollutant concentration plot as parallel straight lines on lognormal graph paper, confirming that concentration is inversely proportional to wind speed and indicating that the standard geometric deviations for these two variables are the same. Pollutant concentrations calculated with a Gaussian multiple-source urban dispersion model also fit lognormality. Calculated and observed cumulative frequency distributions in one study plotted as parallel straight lines and were within a factor of two of each other for almost all of the 40 sites studied.

Factor analysis, eigenvectors, adaptive pattern classification, and various empirical approaches have simplified the characterization and prediction of air pollutant concentration as a function of meteorologic and other variables.

KEY WORDS: air pollutant concentrations, frequency distributions, lognormal, wind speed, diffusion, pattern analysis.

AIR QUALITY FREQUENCY DISTRIBUTIONS AND METEOROLOGY

by Ralph I. Larsen, Ph.D.

Ambient air quality data need to be analyzed to determine if ambient air standards are being violated; if standards are being violated, diffusion and other models can be used to determine various strategies of emission reductions that would achieve the standards.

Ambient air quality data at a given location can be described by a frequency distribution. The purpose of this review is to discuss concentration frequency distributions and compare measured distributions with those calculated by simple and complex meteorologic models.

CONCENTRATION FREQUENCY DISTRIBUTIONS

Ambient air pollutant concentrations are a time function of the strength, height, and distribution of pollutant sources and meteorologic variables such as stability and wind speed and direction. The concentration frequency distribution measured near isolated point sources is highly skewed, with the mode at or near zero. The concentration frequency distribution measured at urban sites is the net result of many sources; it is also skewed, but usually is flatter and has a higher mode.

Several investigators have proposed various mathematical functions to describe these skewed distributions: exponential, chi-squared, logarithmic, lognormal, poisson, negative binomial, gamma (1), beta, and others. Gifford (2,3) has derived mathematical relationships among several proposed frequency functions and has emphasized the broad agreement among the superficially different results.

LOGNORMAL DISTRIBUTION

INVERSE WIND SPEED

Benarie (4,5) has plotted cumulative frequency distributions of inverse wind speed and sulfur dioxide concentration (measured near a point source) on lognormal graph paper. The two plots fit lognormality quite well. They also parallel each other, suggesting that concentration is inversely proportional to wind speed (which fits the expected physical model) and that both parameters have the same standard geometric deviation.

Knox and Lange (6) and Knox and Pollack (7) studied inverse wind speed and carbon monoxide concentration in San Francisco and also noted that the frequency distributions for these two variables paralleled each other when plotted on lognormal paper. They showed that the constant relating the two distributions could be determined either experimentally or with a numerical simulation model.

GAUSSIAN DISPERSION

Turner (8) used a computerized Gaussian dispersion model to calculate and plot (on a lognormal plot) 2-hour (at 10 sites) and 24-hour (at 40 sites) sulfur dioxide concentration cumulative frequency distributions for St. Louis, Missouri, for December, 1964, through February, 1965. He also plotted the measured sulfur dioxide concentration distributions for each site. Both the calculated and measured concentrations fitted lognormality quite well. In many cases the two distributions fell almost on top of each other. In most cases the two distributions were close to parallel and within a factor of two of each other.

AVERAGING TIME MODEL

Larsen (9,10) analyzed 7 years of continuous air pollutant concentration measurements for 7 pollutants (carbon monoxide, total hydrocarbons, nitric oxide, nitrogen dioxide, nitrogen oxides (NO + NO2), oxidant, and sulfur dioxide) in downtown Los Angeles and at the 7 Continuous Air Monitoring Program (CAMP) sites operated by the United States Environmental Protection Agency (EPA) in downtown Chicago, Cincinnati, Denver, Philadelphia, St. Louis, San Francisco, and Washington. He determined cumulative frequency distributions for non-overlapping averaging time periods from 5 minutes to 1 year (Tables 1 and 2; the last 9 columns of the last 6 lines of Table 2 are a summarization of Table 1). All averaging time periods began at midnight. The 8-hour averages were thus midnight to 8 a.m., 8 a.m. to 4 p.m., and 4 p.m. to midnight on one day, midnight to 8 a.m., 8 a.m. to 4 p.m., and 4 p.m. to midnight on the next day, and so on.

Table 1 CONCENTRATION (ppm) VERSUS AVERAGING TIME AND FREQUENCY FOR SULFUR DIOXIDE, WASHINGTON, D.C., DECEMBER 1, 1961, TO DECEMBER 1, 1968

Averaging time	Arithmetic mean	Max	Min	Percent data	Percent of time concentration is equaled or exceeded																
					0.001	0.01	0.1	1	10	20	30	40	50	60	70	80	90	99	99.9	99.99	99.999
5 min	0.05	0.87	0.00	70	0.85	0.49	0.35	0.21	0.10	0.07	0.06	0.04	0.03	0.02	0.02	0.01	0.00	0.00	0.00	0.00	0.00
10	0.05	0.72	0.00	70	0.66	0.47	0.36	0.21	0.11	0.08	0.06	0.04	0.03	0.03	0.02	0.01	0.00	0.00	0.00	0.00	0.00
15	0.05	0.68	0.00	70		0.47	0.35	0.21	0.10	0.07	0.06	0.04	0.03	0.02	0.02	0.01	0.00	0.00	0.00	0.00	
30	0.05	0.68	0.00	70		0.46	0.35	0.21	0.10	0.08	0.06	0.04	0.03	0.02	0.02	0.01	0.00	0.00	0.00	0.00	
1 hr	0.05	0.62	0.00	70		0.45	0.34	0.21	0.10	0.07	0.06	0.04	0.03	0.02	0.02	0.01	0.00	0.00	0.00	0.00	
2	0.05	0.55	0.00	70			0.32	0.21	0.10	0.08	0.06	0.04	0.03	0.03	0.02	0.01	0.00	0.00	0.00		
4	0.05	0.41	0.00	70			0.29	0.20	0.10	0.08	0.06	0.05	0.03	0.03	0.02	0.01	0.01	0.00	0.00		
8	0.05	0.35	0.00	71			0.26	0.18	0.10	0.08	0.06	0.05	0.04	0.03	0.02	0.01	0.01	0.00	0.00		
12	0.05	0.30	0.00	72			0.25	0.18	0.10	0.08	0.06	0.05	0.04	0.03	0.02	0.01	0.01	0.00	0.00		
1 day	0.05	0.25	0.00	72				0.16	0.10	0.08	0.06	0.05	0.04	0.03	0.02	0.01	0.01	0.00			
2	0.05	0.22	0.00	68				0.14	0.10	0.08	0.06	0.05	0.04	0.03	0.02	0.01	0.01	0.00			
4	0.05	0.18	0.00	71				0.14	0.09	0.08	0.06	0.05	0.04	0.03	0.02	0.01	0.01	0.00			
7	0.05	0.13	0.00	73					0.09	0.08	0.06	0.05	0.04	0.03	0.02	0.02	0.01				
14	0.05	0.13	0.00	74					0.09	0.08	0.06	0.05	0.04	0.03	0.02	0.02	0.01				
1 mo	0.06	0.11	0.00	76					0.09	0.08	0.06	0.05	0.04	0.03	0.02	0.02	0.01				
2	0.04	0.10	0.01	74					0.08	0.08	0.06	0.04	0.04	0.03	0.02	0.02	0.01				
3	0.05	0.10	0.01	82						0.07	0.06	0.05	0.04	0.03	0.02	0.02					
6	0.04	0.08	0.01	93							0.06	0.05	0.04	0.04	0.03						
1 yr	0.05	0.05	0.04	86									0.04								

The data showed three characteristics.

First, the cumulative frequency distributions for these pollutants for these averaging times tended to fit lognormality and thus plotted as an approximately straight line on lognormal graph paper (Figure 1 is a plot of Table 1, line 5). The fit was especially good for the high half of air pollutant concentrations of interest in air pollution control.

Second, the median concentrations for the various averaging times tended to plot as a straight line on logarithmic graph paper (50 percentile line on Figure 2; the data listed in Table 1 are the points plotted on this figure). Median concentrations are thus proportional to averaging time raised to an exponent.

Table 2 SULFUR DIOXIDE CONCENTRATION (ppm) AT CAMP SITES, BY AVERAC[illegible] AND FREQUENCY, 1962 THROUGH 1968

City and averaging time	Annual maximum	1962 through 1968				Maximum for year							Percent data available	Per[illegible]ncentration is exceeded							
		Geom. mean	SGD[a]	Max	Min	1962	1963	1964	1965	1966	1967	1968		0.01	[illegible]	[illegible]	[illegible]	30	50	70	90
CHICAGO																					
5 min	3.27	0.104	2.19	1.94	1.11	1.13	1.94	1.62	1.59	1.11	1.62	1.33	83	1.31	[illegible]	[illegible]	[illegible]	0.16	0.08	0.03	0.01
1 hr	1.98	0.112	2.00	1.89	0.86	0.86	1.89	1.12	1.14	0.98	1.11	0.91	83	1.11	0.95	0.64	0.32	0.16	0.08	0.03	0.01
8 hr	0.86	0.118	1.84	1.02	0.45	0.45	0.87	1.02	0.74	0.63	0.80	0.63	84		0.74	0.36	0.31	0.16	0.09	0.04	0.01
1 day	0.63	0.121	1.75	0.79	0.36	0.36	0.71	0.79	0.55	0.48	0.65	0.51	86			0.49	0.30	0.16	0.09	0.05	0.02
1 mo	0.24	0.133	1.44	0.35	0.18	0.18	0.33	0.35	0.27	0.26	0.32	0.26	94				0.27	0.18	0.09	0.06	0.03
1 yr	0.14	0.142	1.00	0.18	0.09	0.10	0.14	0.18	0.13	0.09	0.12	0.12	100						0.12		
CINCINNATI																					
5 min	1.68	0.016	2.87	1.49	0.65	0.84	0.99	0.88	1.15	0.70	0.66	1.49	80	0.68	0.41	0.19	0.06	0.03	0.02	0.01	0.00
1 hr	0.65	0.018	2.54	0.57	0.39	0.46	0.48	0.55	0.57	0.41	0.42	0.38	80	0.53	0.33	0.18	0.06	0.03	0.02	0.01	0.00
8 hr	0.30	0.020	2.27	0.38	0.14	0.14	0.23	0.27	0.38	0.18	0.18	0.18	81		0.22	0.12	0.06	0.03	0.02	0.01	0.00
1 day	0.20	0.022	2.12	0.18	0.08	0.11	0.11	0.14	0.18	0.10	0.13	0.08	82			0.10	0.06	0.04	0.03	0.02	0.01
1 mo	0.06	0.025	1.63	0.06	0.03	0.04	0.06	0.06	0.06	0.05	0.04	0.03	86				0.05	0.03	0.03	0.02	0.01
1 yr	0.03	0.029	1.00	0.04	0.02	0.03	0.03	0.04	0.03	0.03	0.02	0.02	100						0.03		
DENVER																					
5 min	0.47	0.013	2.28	1.81	0.33				0.95	0.96	0.33	1.81	78	0.38	0.16	0.08	0.03	0.02	0.01	0.00	0.00
1 hr	0.22	0.014	2.07	0.36	0.17				0.36	0.26	0.17	0.24	78	0.26	0.13	0.07	0.03	0.02	0.01	0.00	0.00
8 hr	0.12	0.015	1.90	0.14	0.05				0.14	0.10	0.05	0.10	79		0.10	0.05	0.03	0.02	0.01	0.00	0.00
1 day	0.09	0.015	1.80	0.07	0.02				0.06	0.05	0.02	0.07	81			0.04	0.03	0.02	0.01	0.00	0.00
1 mo	0.03	0.017	1.46	0.03	0.01				0.03	0.02	0.01	0.03	83				0.02	0.02	0.01	0.01	0.00
1 yr	0.02	0.018	1.00	0.02	0.01				0.02	0.01		0.01	100						0.01		
LOS ANGELES																					
5 min	0.47	0.013	2.28	0.68	0.24	0.24	0.51	0.68					59	0.38	0.15	0.08	0.04	0.02	0.01	0.01	0.00
1 hr	0.22	0.014	2.07	0.29	0.13	0.13	0.19	0.29					67	0.25	0.13	0.08	0.04	0.02	0.01	0.01	0.00
8 hr	0.12	0.015	1.90	0.13	0.08	0.08	0.09	0.13					71		0.10	0.07	0.04	0.02	0.02	0.01	0.00
1 day	0.09	0.015	1.80	0.10	0.06	0.06	0.07	0.10					71			0.06	0.04	0.02	0.02	0.01	0.00
1-mo	0.03	0.017	1.46	0.03	0.02	0.03	0.03	0.02					64				0.02	0.02	0.02	0.01	0.01
1 yr	0.02	0.018	1.00	0.02	0.02	0.02	0.02						67						0.02		
PHILADELPHIA																					
5 min	2.67	0.055	2.41	1.25	0.79	1.25	1.05	1.00	1.11	0.79	1.12	1.10	77	0.96	0.72	0.48	0.20	0.08	0.05	0.03	0.01
1 hr	1.19	0.060	2.18	1.03	0.66	1.03	0.85	0.84	0.94	0.66	0.77	0.88	78	0.85	0.67	0.45	0.20	0.09	0.05	0.03	0.01
8 hr	0.81	0.064	1.99	0.71	0.43	0.56	0.58	0.54	0.71	0.43	0.56	0.55	79		0.52	0.37	0.19	0.10	0.06	0.04	0.01
1 day	0.43	0.067	1.88	0.46	0.35	0.35	0.46	0.43	0.35	0.36	0.35	0.36	81			0.31	0.17	0.10	0.07	0.04	0.02
1 mo	0.15	0.075	1.50	0.16	0.12	0.13	0.12	0.15	0.13	0.13	0.13	0.16	88				0.12	0.10	0.08	0.07	0.04
1 yr	0.08	0.081	1.00	0.10	0.06	0.09	0.08	0.09	0.08	0.09	0.10	0.08	100						0.08		
ST. LOUIS																					
5 min	2.32	0.028	2.72	1.42	0.85			1.18	1.47	1.25	0.85	1.33	83	0.94	0.56	0.28	0.10	0.04	0.02	0.01	0.00
1 hr	0.84	0.032	2.43	0.86	0.55			0.73	0.86	0.84	0.55	0.68	83	0.73	0.49	0.25	0.10	0.05	0.02	0.01	0.00
8 hr	0.44	0.034	2.18	0.36	0.23			0.31	0.36	0.33	0.24	0.23	84		0.29	0.18	0.09	0.06	0.03	0.02	0.00
1 day	0.30	0.036	2.05	0.26	0.16			0.26	0.19	0.18	0.21	0.16	86			0.14	0.08	0.05	0.03	0.02	0.01
1 mo	0.09	0.042	1.59	0.08	0.05			0.08	0.06	0.06	0.05	0.06	90				0.06	0.06	0.04	0.03	0.01
1 yr	0.05	0.047	1.00	0.06	0.03			0.06	0.06	0.04	0.03	0.03	100						0.03		
SAN FRANCISCO																					
5 min	0.56	0.005	2.87	0.33	0.16	0.16	0.33	0.26					64	0.16	0.13	0.07	0.03	0.01	0.01	0.00	0.00
1 hr	0.22	0.006	2.54	0.26	0.11	0.11	0.26	0.16					64	0.16	0.11	0.07	0.03	0.01	0.01	0.00	0.00
8 hr	0.10	0.007	2.27	0.10	0.06	0.06	0.07	0.10					65		0.09	0.06	0.03	0.02	0.01	0.00	0.00
1 day	0.07	0.007	2.12	0.08	0.05	0.06	0.05	0.08					66			0.05	0.03	0.02	0.01	0.00	0.00
1 mo	0.02	0.008	1.63	0.03	0.01	0.01	0.02	0.03					75				0.02	0.01	0.01	0.01	0.00
1 yr	0.01	0.010	1.00	0.02	0.01		0.01	0.02					67						0.01		
WASHINGTON																					
5 min	1.14	0.040	2.14	0.87	0.42	0.42	0.58	0.87	0.44	0.47	0.44	0.53	70	0.49	0.35	0.21	0.10	0.08	0.03	0.02	0.00
1 hr	0.56	0.042	1.96	0.62	0.35	0.38	0.48	0.62	0.35	0.45	0.37	0.42	70	0.45	0.34	0.21	0.10	0.06	0.03	0.02	0.00
8 hr	0.31	0.045	1.81	0.35	0.22	0.23	0.25	0.32	0.27	0.34	0.22	0.22	71		0.26	0.18	0.10	0.06	0.04	0.02	0.01
1 day	0.23	0.048	1.72	0.25	0.15	0.18	0.25	0.22	0.20	0.25	0.15	0.18	72			0.16	0.10	0.06	0.04	0.02	0.01
1 mo	0.09	0.050	1.42	0.11	0.07	0.10	0.11	0.09	0.08	0.10	0.07	0.10	76				0.09	0.06	0.04	0.02	0.01
1 yr	0.06	0.053	1.00	0.05	0.04	0.05	0.05	0.04	0.05	0.04		0.04	86						0.04		

[a] Standard geometric deviation.

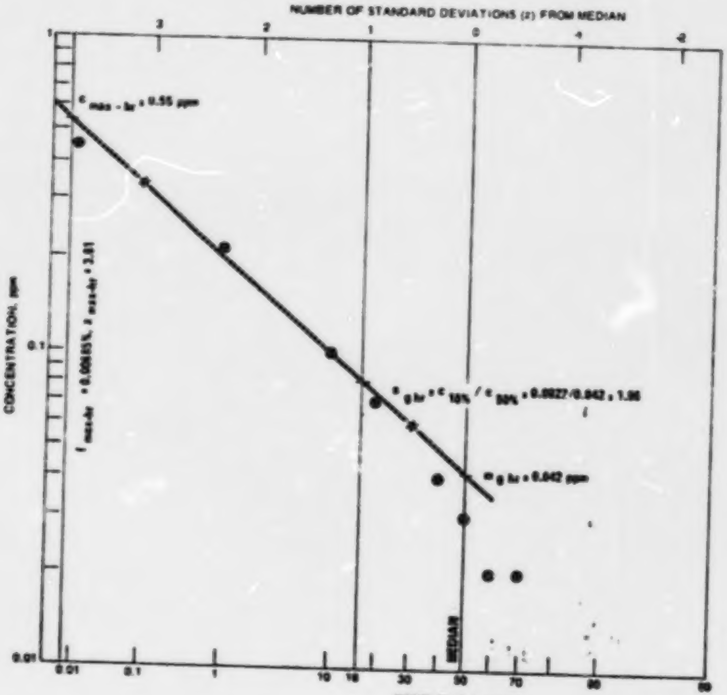

Figure 1. Frequency of 1-hour-average sulfur dioxide concentrations equal to or in excess of stated values, Washington, D.C., December 1, 1961, to December 1, 1968.

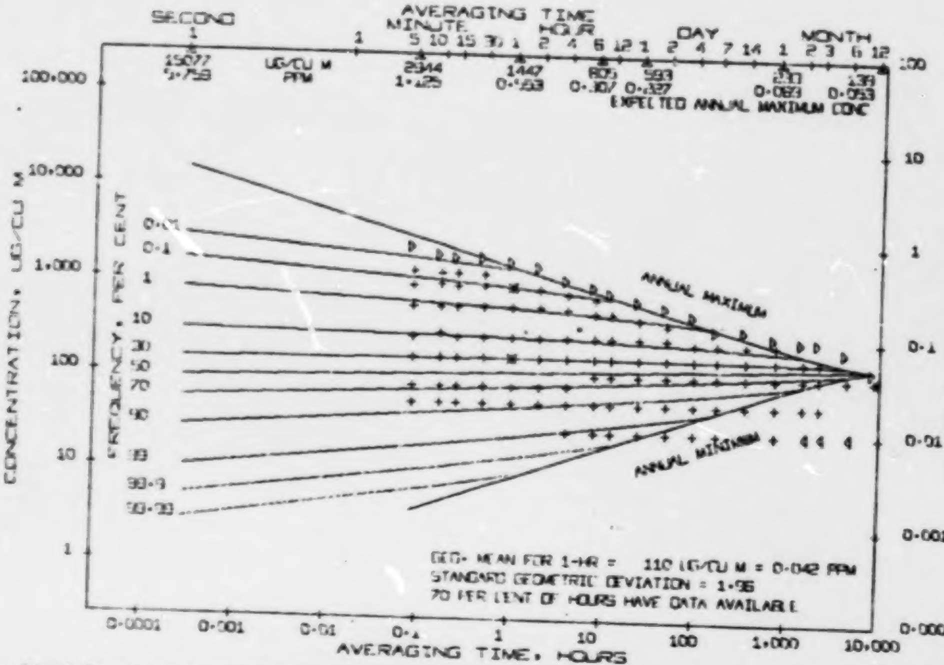

Figure 2. Computer plot of concentration versus averaging time and frequency for sulfur dioxide at site 256, Washington, D.C., December 1, 1961, to December 1, 1968.

Third, maximum concentrations also tended to plot as a straight line (top line on Figure 2). Maximum concentrations are thus approximately inversely proportional to averaging time raised to an exponent.

An empirical mathematical model incorporating these three characteristics of pollutant concentration has been developed. It is helpful for comparing observed pollutant concentrations with air quality standards and for calculating statistical properties of pollutant concentrations for various averaging times. The resulting information can be used in developing implementation plans and emission standards. It is especially helpful for determining the overall average source reduction needed to achieve an air quality standard.

The above averaging time model uses the lognormal distribution to calculate maximum concentrations expected to occur an average of once a year. These values can be compared with the United States National ambient air standards that specify concentrations that are not to be exceeded more than once a year. Singpurwalla (11) and Barlow and Singpurwalla (12) have used extreme value theory to calculate these maxima.

PATTERN ANALYSIS

Forecasts of daily sulfur dioxide concentrations can be used to predict air pollution episodes and the possible need for hospital beds. Smith and Jeffrey (13) analyzed sulfur dioxide concentration as a function of meteorology in London and Manchester in order to make such forecasts. They used observed data to develop an empirical relationship and an easy-to-use nomogram (Figure 3) to forecast daily sulfur dioxide concentration as a function of minimum temperature, hours of calm, concentration on previous day, low or high wind speed, wind direction in one of two sectors, and low or high mixing height.

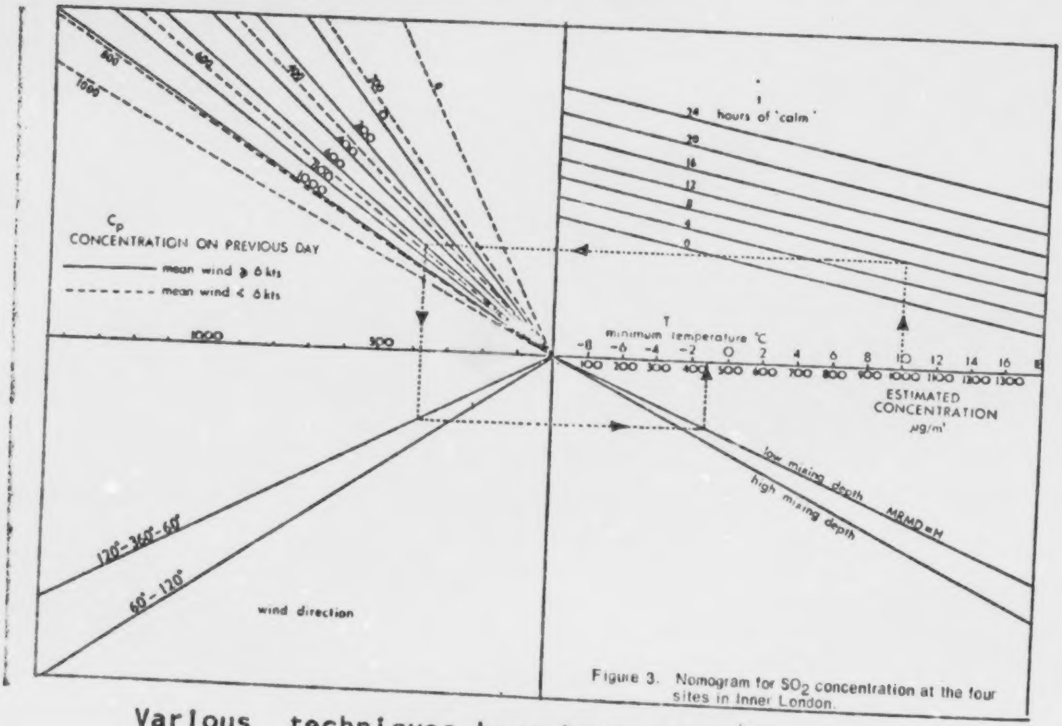

Figure 3. Nomogram for SO_2 concentration at the four sites in Inner London.

Various techniques have been used to determine which independent variables explain most of the variation in air pollutant concentrations. The selection of the few most important variables simplifies the expression of air quality as a function of meteorology. Prinz and Stratmann (14) used factor analysis for this purpose.

Peterson (15,16) used eigenvectors to characterize the pattern of 24-hour mean sulfur dioxide concentrations at 30 locations in St. Louis, Missouri, on 49 days during the winter of 1964-1965. The first three derived patterns explained two-thirds of the variance.

Adaptive pattern classification is a computer oriented technique to calculate the value for a categorized dependent variable as a function of a set of input variables, called a pattern. Ruff (17) used this technique to study the production of ozone in the San Francisco Bay Area as a function of other pollutant and meteorologic variables.

SUMMARY

Cumulative frequency distributions of the following three variables tend to plot as parallel straight lines on lognormal graph paper: (1) inverse wind speed, (2) air pollutant concentrations for urban multiple-source emissions calculated with a Gaussian dispersion model at a given location, and (3) measured air pollutant concentrations at the same location. This suggests that these variables are proportional to each other and are lognormally distributed.

Factor analysis, eigenvectors, adaptive pattern classification, and various empirical approaches simplify the calculation of air pollutant concentration as a function of meteorologic and other variables.

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Chapter XVI

THE SIMPLE ATDL URBAN AIR POLLUTION MODEL

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Introduction

I would like to use the time at my disposal to describe the simple urban air pollution model in use at ATDL, Oak Ridge, to review briefly some of our experience with applications and validation of this model, and to discuss a little bit our philosophy of air pollution modelling. It is by no means the least virtue of such a simple model as I will describe that it leaves some time for data comparisons and consideration of the broader philosophy of the subject. Before describing the model let me say that in my mind "simple" is the opposite not of "sophisticated" but of "complex". The antonym of "sophisticated" is, I think, "naive". I hope to be able to convince you that simple urban pollution models are not necessarily naive, and may in fact represent the essence of sophistication, in the better sense of that word.

The ATDL Simple Urban Dispersion Model

Direct ATDL involvement with urban diffusion modelling began in 1969 when we were asked to calculate the potential atmospheric concentration of tritiated natural gas in the Los Angeles basin[1], as part of the USAEC's Project Plowshare. Of course we had been thinking about the urban pollution problem for a number of years, and had come to several conclusions about it. First it seemed clear that urban air pollution concentration at any point could be influenced by sources in a narrow, plume-shaped upwind sector only[2]. This means that one doesn't have to consider all the sources in the entire semi-infinite upwind half-plane.

Second, the usual urban source-inventory grid pattern is of the order of 5 km on a side, rarely less. This is much larger than the width of a typical plume. Consequently as a practical matter it seemed that the variation in the cross-wind direction of the source-strength pattern could be ignored, at least for receptors within a city. Consequently the urban area-source pollution problem seemed in several important ways to be conceptually far simpler than the point-source problem[3].

The area-source model that we adopted based on these simplifications turns out to involve just an integration in the upwind direction of a cross-wind infinite line-source diffusion formula. In practice we use the Gaussian version, but this point makes little difference; K-theory line-source formulas could be used just as well, or other formulations, i.e. those based on Lagrangian similarity theory. The results should tend not to be very sensitive to the particular diffusion model employed, since only the vertical diffusivity is involved, according to our simplifications. Furthermore only the surface-level concentration needs to be calculated, not its vertical distribution. And since receptors are located as a rule within the city, they will tend to be little affected by remote pollution sources. Thus a simple power-law expression for the vertical diffusivity is quite adequate, e.g. $\sigma_z = ax^b$, because this expression need only work to fairly modest values of the distance, x, between source and receptor. A brief mathematical summary is given in the Appendix to this note.

Based on this line of reasoning, we argued[4] that the area-source component of a stable, non-reacting pollutant species would be adequately described by the following formula:

$$X = \left(\frac{2}{\pi}\right)^{1/2} \frac{(\Delta x\ /2)^{1-b}}{a(1-b)\ U} \left\{ Q_o + \sum_{i=1}^{N} Q_i \ [(2i + 1)^{1-b} - (2i - 1)^{1-b}] \right\} \qquad (1)$$

where X is the pollutant concentration at ground level, U is the mean wind speed, Δx is the source inventory grid spacing, and Q_i are the source inventory strengths in the $(N + 1)$ upwind source boxes, $i = 0, 1, \ldots, N$. The total ambient air quality follows from summing the contributions of eq. (1), together with the point sources and the background contribution. Though our rationale was, I believe, a considerable step forward, equation (1) is closely related to several area source formulas based on the Gaussian model, particularly the study by Clarke[5]. We showed[4] that calculations based on equation (1) did not differ substantially from results based on far more complex mathematical models. Also comparisons with observed air pollution data averaged over periods ranging from 1 hour to 1 year were made.

Based on many comparisons of this kind, Hanna[6] concluded that the following simpler model

$$X = C\ Q_o/U \qquad (2)$$

where C = constant, might work just as well. From (1) and (2)

$$C = (2/\pi)^{1/2}[(2N + 1)\ \Delta x/2]^{1-b} \cdot \ [a(1 - b)]^{-1} \ . \qquad (3)$$

Equation (1) can be thought of as a box-model the height of whose lid increases downwind according to equation (3). The assumption $Q_i = Q_o$ is valid because source strengths mostly do not vary rapidly over the source-grid squares, which are in any case large. Since the quantity (1 - b) is a fairly small fraction, and the product a(1 - b) varies slowly in the stability range ordinarily encountered over cities, the assumption that C = constant for a given stability condition is quite reasonable. Our experience is that C can be assigned the approximate values 50, 200, and 600 for unstable, neutral, and stable conditions.

Comparisons with Air Pollution Data

Equation (2) was calibrated by means of annual air pollution data from 44 U.S. cities and the constant C determined to average approximately 225 for non-reacting pollutants. Comparisons of equation (2) with various more detailed pollution models show that it is a consistently better predictor of long-term air-pollution patterns[7]. The model has also been compared with annual particle pollution mean values, with annual and seasonal SO_2 and particle pollution patterns[7], with short term pollution patterns down to 1 hour[6], with time varying CO pollution patterns up to 48 hours[8], and with photochemical pollution[13].

Equation (2) has been compared, in these references, with a very much larger quantity of air pollution data than has any other model. In these comparisons it consistently equals or outperforms more complex models. Table 1 summarizes these results.

Table 1

Comparison of Simple ATDL Urban Pollution Model With Various Other Models

City	Concentration value modelled	Period	Pollutant	Correlation Coefficient		Model	Reference
				ATDL	Other		
Chicago	Point	24 hr (for 18 days)	SO_2	.67	.69	Roberts, *et al*.	6
Chicago	Point	6 hr (for 4 days)	SO_2	.66	.80	"	6
Memphis	Area Pattern	Annual	Particle	.68	.73	AQDM	7
Nashville	"	"	"	.91	.80	"	7
Ankara	"	Seasonal	"	.63	.59	CDM	7
Bremen	"	"	SO_2	.65	.05	Fortak	7
"Test City"	"	Annual	Particle	.98	.96	AQDM	7
L.A.	Point	1 hr (for 17 hrs)	CO	.89	.48	PICK	8
San Francisco	"	1 hr (for 48 hrs)	"	.74	.66	McCracken *et al*.	8
L.A.	Area Average	1 hr (for 7 hrs)	NO	.97	.91	PICK	13
"	"	"	NO_2	.05	-.42	"	13
"	"	"	Reactive Hydrocarbons	.61	.55	"	13
London	"	24 hr avg.	SO_2	.76	.87	Met. Office	14

For all cases where verification data in the form of observed concentration values are available, the (linear) correlation coefficient between these and values calculated from the simple ATDL model and those calculated by the various other models are listed. In interpreting these correlations it should be kept in mind that the level of this number in any particular case is strongly affected by such things as placement of air pollution sampling stations. Also in many instances the number of samples available for correlation is quite small. Consequently the correlation value is not by itself a very good measure of the efficiency of any particular modelling scheme. However the difference between any pair of correlations, and in particular the consistency with which this difference is repeated over nearly all the pairs, is a convenient and valid criterion for comparing models.

You may be interested in one further comparison, with the daily SO_2 concentrations for Rotterdam, as published in the 3rd (Paris) meeting of this panel. Daily values of SO_2 averaged over 31 stations in the Rotterdam area for 19 days, Sept. 16 to Oct. 4, 1971 were included in the paper by Velds[9]. For this situation our model would predict a variation in average urban SO_2 concentrations with U^{-1}, assuming that the average source was constant during that period. In the following table there are correlations of concentration values with various of the meteorological quantities published by Velds (see his Table 1):

Table 2

Correlation of daily mean SO_2 Conc. with:		Correlation Coefficient
1/U	:	.6
Max. mixing height	:	.1
Mixing height at T+1 hr. (col.2)	:	.1
Daily persistence (correlation with previous day's value)	:	.3

As an example of such data comparisons with equation (2), Table 2 is about run-of-the-mill. It shows, as we would expect, that most of the day-to-day variability in SO_2 concentration comes from mean wind speed variability (assuming no source variability). Of course there is in autumn most likely a positive correlation between SO_2 emissions and U, which might have improved the overall performance of our model if source data were available. The correlation .6 is by itself not, as was mentioned earlier, necessarily especially meaningful; but there seems to be a significant improvement over persistence. Dr. Velds concluded, from the same data, that "probably it will be impossible to use a mathematical model" in this case. It would be interesting to have the benefit of his comment on exactly what mathematical models he has actually tested with these data, and what the results were.

A final point on this comparison concerns the low correlation with mixing height exhibited in Table 2. This result, which seems superficially to be at odds with so much of current thinking on urban air pollution meteorology, has been found by my colleague Dr. Hanna and me in several cases, in fact wherever we have been able to get data. The reason seems to be that the vertical growth of the urban pollutant cloud from a given differential source area (or "point") is small compared with the usual mixing depth over a receptor point. From equation (3), since $\sigma_z = ax^b$, it follows that

$$C \approx x/\sigma_z \quad . \tag{4}$$

Recall that x/σ_z is on the order of 200. Thus by the time σ_z has grown to 500 or 1000 m, the usual range of mixing depths, the corresponding distance x from source to receptor averages 200 times that; and sources much nearer the receptor point are dominating the ambient air quality.

It should perhaps also be pointed out that combining equations (4) and (2) gives

$$X/Q_o = (1/\sigma_z)\ (x/U) \quad . \tag{5}$$

The quantity U/x is essentially what Lettau[10] terms the "flushing frequency," in his very elegant exposition of the role of the box model of urban diffusion.

Concluding Remarks

It is probably not necessary to point out to this group that equation (2) can easily be combined with wind or stability climatological frequency distributions to build up pollution frequency distributions. Also simple exponential removal processes such as washout, or radioactive or chemical decay, are readily introduced without complication[11]. The more difficult problem of urban pollution with a complex chemical reaction scheme, such as photochemical smog, can also be greatly simplified and systematized with the help of equation (2) as Hanna has shown[12,13]. Here again the (in this case extremely meagre) experimental data indicate better agreement from the resulting simple, than from more complex models. Obviously more comparisons, involving optimized chemical reaction schemes as well as more extensive real-world (as opposed to laboratory) air pollution data, need to be made in this area. We have every confidence that such comparisons will continue to demonstrate the durability and utility of the simple model.

I would like to emphasize the last sentence. Although we started out only to develop the simplest urban air pollution model that would do a reasonably good job, our studies have inexorably led us to the following conclusion. The simple model consistently gives slightly better results than more complex models. Not just "about as good," but "slightly better." The difference is not great but it is rather consistent and of course leads to the question, "Why?" We do not consider it to be part of our job to give a detailed answer to this question. Indeed to do so would require close study of a fairly large number of very complex urban pollution modelling studies, the details of many of which have not all been published just because of their great complexity.

I would like, however, to suggest two points. First of all, we don't believe, any more than you do, that there has been any failure either of the applicability of basic physical theory or of the application of mathematical techniques, i.e. of "sophistication," in the complex models. Rather, if there has been a failure, it is one of pushing on too rapidly with theoretical modelling without adequate experimental checks against the real atmosphere. That is, it is a question of "naivety" that is involved. Secondly, there is the problem of how urban pollution modelling is to be improved. Apart from the influence of chemical reactions and removal processes, the main factors are again, we believe, displayed in equations (2) or (5). Namely it seems clear that the gross influences of variations of source strength, mean wind transport, and stability, which are the basics of atmospheric pollution as Lettau[10] pointed out, must be accounted for first, and only then other effects.

Appendix

With notation similar to that employed in Calder's formulation of the problem, the concentration $X_A(x,y,z)$ at or above any receptor point (x,y) due to a distributed, area source can be expressed as follows;

$$X_A(x,y,z) = \int_{-\infty}^{\infty} \int_{-\infty}^{x} Q(x_o,y_o,z_o)\ R(x-x_o,y-y_o,z)\ dx_o\ dy_o \qquad (1)$$

$R(x,y,z)$ is a continuous point source concentration function and $Q(x_o,y_o,z_o)$ is the area source distribution function. The area source strength Q can be regarded as a continuously varying function of x_o and y_o or a discontinuous function; z_o is, mostly as a matter of convenience, assigned a particular value (often zero). That is, the effective height of the area source is usually handled as a parameter of the problem.

Equation (1) assumes a quasi-steady state, i.e. that at least over some reasonable period of averaging the meteorological and source conditions are not changing rapidly with time. More complex states are synthesized from these steady periods. The continuity condition for a single continuous point source then requires that

$$\int_{-\infty}^{\infty} \int_{0}^{\infty} U(z) R(x-x_o,y-y_o,z) dz\ dy_o = 1. \qquad (2)$$

If Eq. (1) is multiplied by $U(z)$, integrated with respect to height, z, above the receptor point, and the order of integrations changed,

$$\int_{0}^{\infty} U\, X_A\, dz = \int_{-\infty}^{x} \int_{-\infty}^{\infty} \int_{0}^{\infty} UR\, Q(x_o,y_o;z_o)\, dz\, dy_o\, dx_o \qquad (3)$$

If $Q = Q(x_o;z_o)$ only, substitution of (2) in (3) would give

$$\int_{0}^{\infty} u\, X_A\, dz = \int_{-\infty}^{x} Q(x_o;z_o)dx_o \quad . \qquad (4)$$

Note that no assumption about the form of the point source function, R, is involved in this argument, only an assumption about the source distribution.

The assumption that Q varies with x_o only (z_o being a parameter) is not particularly restrictive. The reason is that concentration in real point-source plumes is observed to decrease very rapidly with lateral distance from the plume centerline. Those sources that influence X_A appreciably will lie in a fairly narrow, plume-shaped upwind sector. The angular width of this sector will depend in theory on the form of R and will be controlled by atmospheric stability; but that it is small as a practical matter is shown by the ordinary, elongated appearance of plumes. The assumption $Q = Q(x_o)$ for the area source function should be closely approximated in this sector except possibly for Q of highly unusual shape. This being the case, equation (4) implies that X_A can in general be expected to be independent of the lateral concentration variation of the distribution function R.

With no loss of generality equation (4) can be rewritten as

$$\int_{0}^{\infty} U(z)\, X_A\, dz = \int_{x_u}^{x} Q(x_o)dx_o \qquad (5)$$

where $x-x_u = D$ is the distance from a receptor to the upwind "edge" of the city. This "edge" could be taken, for instance, to be the upwind point where rural background or some other standard value of concentration is reached. Equation (5), a continuity equation for area source pollution, is a statement of the fact that the total flux of pollutants through a vertical column equals the upwind source strength. It can be rewritten in the form

$$\int_0^\infty U(z)X_A(z)dz = D\bar{Q} \qquad (6)$$

using the ordinary definition of a mean value. That is, for any given upwind source configuration, there exists some mean value, $\bar{Q}$.

The area source pollution problem also must satisfy an appropriate differential equation. According to the simplifications introduced previously, this will be the steady-state, one-dimensional diffusion equation,

$$U(z)\ \partial X_A/\partial x = \partial/\partial z\ (K_z(z)\ \partial X_A\ /\partial z) \quad . \qquad (7)$$

Solutions to (7) for line-source boundary conditions and assuming power-law variation of U(z) and K(z) have been summarized by Pasquill[16]. These solutions are rather complex; but the essential properties involved in the area-source problem can be brought out by the following alternative line of reasoning.

Assuming the usual power law forms

$$U(z) = U_1(z/z_1)^m \qquad (8)$$

and

$$K_z(z) = K_1(z/z_1)^n \qquad (9)$$

We can look for a variables separable solution to the area-source problem of the form

$$X_A = X_{AO}\,(x)\; f\,(x,z) \quad . \tag{10}$$

This is found by introducing the independent variable transformation $\zeta = z/Z(x)$, and then determining Z so that equations (7) - (10) are satisfied. The required condition on Z turns out to be

$$Z(x) = c_1 x^{\,1/(2+m-n)} \tag{11}$$

Equations (8), (10), and (11), which resulted from considering the differential equation (7), are now introduced into the integral condition, equation (6), and the result solved for X_{AO}, the desired, ground-level concentration:

$$X_{AO} = \frac{D\,\bar{Q}}{U(Z)Z(D)B} \quad . \tag{12}$$

The quantity B is a constant parameter, defined by

$$B = \int_0^\infty \zeta^m\, f(\zeta)\, d\zeta \quad . \tag{13}$$

Apart from the unknown constant c_1 in the definition of Z, the undetermined quantities of this solution are all incorporated into the constant B.

Equation (12) is the basis for the simple ATDL urban diffusion model. In practice, in order to estimate B and c_1, we have assumed that R, in equation (1), has the usual Gaussian form. In this case equation (12) above reduces to equations (1) - (3) of the text, and it is easily shown that $b = 1$ and $c_1\,B = a(1-b)(\pi/2)^{1/2}$. (The parameters a and b for various atmospheric stability conditions can be found for instance in reference 4.)

Notice also that both Z and thus U in equation (12) depend on D only; that is they are constants for any given stability condition and receptor location. As we have previously pointed out[4], the variability with receptor location (city size) is quite small. Variability with atmospheric stability also tends to be small because of the generally small range of stability conditions encountered over a city. Finally U/D can be identified with the "flushing frequency" and UZ/D is a "flushing velocity," in the terminology introduced by Lettau[10].

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Chapter XVII

Real-Time Meteorological Prediction in Support of Air-Quality Control Operations in Canada

4th Meeting of NATO/CCMS Panel on Modeling

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Real-time Meteorological Prediction in Support of Air-Quality Control Operations in Canada (Including Regional Air Pollution Model Development)

1. Purpose

These comments describe the kind of routine meteorological forecast support that can be provided for air pollution episode control activities and it indicates how current programs and plans of the Atmospheric Environment Service (AES) relate to such support.

2. The AES Weather Forecasting System

In order to appreciate the capabilities of the Atmospheric Environmen Service in this area, it is necessary to gain an adequate understanding of the nature and scope of the Canadian operational Weather Forecasting System. This Forecast System is part of a large international integrated co-operative entity which is known as World Weather Watch (WWW). The Canadian national system has the following main components: (a) an observational system, (b) a complex national weather communications system (teletype and facsimile) (c) a Canadian Meteorologic Centre in Montreal with numerical weather prediction capability (with a staff of more than 100 people and a very large computer facility), (d) about a dozen forecast offices scattered across the country, plus a number of auxiliary service outlets, (e) a substantial R & D program to back up the operational system.

The system operates 365 days a year observing, processing and transmitting on a minute-by-minute and hour-by-hour basis real time services to a multitude of users. Users are able to negotiate with AES for teletype and facsimi drops from local offices to have access in real-time to various prediction product of interest to them.

A program is proceeding to computerize and automate many of the routine procedures at the forecast offices and this will permit a substantial proliferation over the next few years in the number and kinds of end products available to users. Because these outputs build on the same basic information and processing base, the add-on costs for even substantial numbers of new products will be very modest.

3. Air Quality Prediction as a Meteorological Problem

Forecasting pollutants in the atmosphere is a normal meteorological problem which, except for new physical and chemical parameters, and processes can be handled by the same theory, procedures and models that are used to predict other meteorological phenomena, namely, the Navier-Stokes equations. A good comparison is with water vapour in the atmosphere which enters from various surface sources, is moved about, changes state and falls out as precipitation. The forecasting of water in the atmosphere is a critically important question in meteorological prediction since, in addition to its role as precipitation, it has a powerful feed back effect on the atmosphere due to the latent-heat of condensation and the impact on atmospheric radiation.

Until very recently, the main air quality prediction problem that has ated interest and study involves the prediction of the near-plant environment. s has resulted in the development of diffusion models while most of the meteorgical controlling factors have been handled independently. With interest in quality expanding to metropolitan, regional and hemispheric scales the approach handling air quality models on a full, meteorological basis is receiving more ention. In such a comprehensive approach the pollutant aspects are no longer add-on to independent meteorological predictions but become an integral part the process.

In terms of AES R & D, procedures to utilize a large spectrum of omated models and methods are being examined for exploitation in terms of quality prediction. The approach permits utilization of the full resources complexities of meteorological prediciton in support of air quality control rations. While the Federal Government for pollutuon abatement follows the cept of "concentrate and contain" applied at the pollution source through use of the best practical technology, the use of meteorological prediction ld greatly assist in using the assimilative capacity of the atmosphere to lute and disperse" the remaining pollutants. Furthermore, the prediction els would identify the areas where pollution abatement might be required in ew years through simulation models.

Current AES Prediction Support for Air Quality

Aside from the prediction of standard meteorological variables (e.g., d, temperature, stability) the major air quality prediction support routinely ilable from the AES at the present time involves forecasts of so-called Stagnation related Indices. These indices give a general qualitative indication of the lity of the atmosphere to move air pollutants vertically or horizontally from ir source regions. This approach has several limitations, (a) the indices do entirely relate to the physical processes involved in the movement of lutants, (b) the method does not give a quantitative measure of the ventilation ability of the atmosphere, (c) it does not take into account local variability to terrain. These indices together with meteorological forecasts are able, ever, to give air quality control agencies general guidance in assessment of risk of build-up of pollutants.

AES R & D Programs in Air Quality Prediction

1 A number of R & D projects are currently underway whose results can be used to provide a variety of air quality forecast aids. Some of these studies have not reached the point where they can be tested against real data. The proposed technology is capable of being upgraded with further study. The projects are listed in order of increasing time to completion. Preliminary versions of the top few are expected to be available for operational testing in the next year or so. Following is a condensed list of the projects.

(a) The development of a relative air-pollution potential index which would give a number, directly relatable to air pollution build-up for specified areas of the scale of 100 km to a side. Initially, these indices would describe a rate of potential build up and be available twice a day. Somewhat later they could be made available on an hourly basis and also describe the accumulated effect on pollutant build-up over any desired time frame up to three days.

(b) With the availability of pollution source parameters (on the scale of the prediction) from source inventories or estimates and the development of special boundary-layer dynamic-numerical models and the introduction of appropriate pollutant transformations and sinks, the indices can be replaced by actual pollution predictions.

(c) Projects which will permit the introduction of terrain influences and special urban models can provide predictions down to a scale of 10 km. These could be used to examine the projected variability over large metropolitan areas or give the predicted build up over smaller metropolitan areas and large industrial complexes. The use of nested grids can result in solutions to a scale of one km or less.

(d) Systems to examine and predict the large-scale background pollution, much of it moving across Canada - U.S.A. boundary, will be developed both to increase the accuracy of local prediction and to study the total hemispheri problem.

5.2 Certain ancillary products or services can be provided by the procedures and models described above:

(a) Information can be provided on the appropriate response to a threatened air pollution incident by rerunning prediction models with alternative source distributions. This could also be helpful where control is exerted by substituting cleaner types of fuel.

(b) On the scale of the forecasts, instances of high pollution intensities can be associated with source regions. This can be useful where terrain plays a major role.

(c) Point values of pollutant concentration can be related to estimated area averages. This would be of particular interest where point values are used for control purposes.

(d) Using climatological mean data as well as typical sets of meteorological conditions the models can be used to deduce pollutant concentration means, extremes and related statistical parameters over various areas for planning purposes. This can be done for any desired projection of pollutan source distributions.

(e) Concentrations and masses of pollutants brought down by precipitation can be calculated to help with planning of land and water use.

A program to study satellite observation of pollution is veing developed in conjunction with U.S. and Canadian satellite plans. Some experimentation with the use of weather satellites to observe large-scale particulate pollution has been started. Such systems seem to have excellent potential for measuring areal averages over squares of a few kilometers to a side or larger. Higher resolution data would be costly to obtain in real time.

6. Summary

The above describes the kinds of real-time support that may be provided by AES forecast systems in the future. The emphasis has been on routine systems and, thus, special studies for examining individual plant or stack criteria or design, special models for planning purposes, studies to improve the background science, climatic impact studies, etc. are not discussed here.

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